Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID: SSSPTA1626GMS

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

```
NEWS 1
                Web Page URLs for STN Seminar Schedule - N. America
NEWS 2
                "Ask CAS" for self-help around the clock
NEWS 3 JUL 20 Powerful new interactive analysis and visualization software,
                STN AnaVist, now available
NEWS 4 AUG 11 STN AnaVist workshops to be held in North America
NEWS 5 AUG 30 CA/CAplus -Increased access to 19th century research documents
NEWS 6 AUG 30 CASREACT - Enhanced with displayable reaction conditions
NEWS 7 SEP 09 ACD predicted properties enhanced in REGISTRY/ZREGISTRY
NEWS 8 OCT 03 MATHDI removed from STN
NEWS 9 OCT 04 CA/CAplus-Canadian Intellectual Property Office (CIPO) added
                to core patent offices
NEWS 10 OCT 06 STN AnaVist workshops to be held in North America
NEWS 11 OCT 13 New CAS Information Use Policies Effective October 17, 2005
NEWS 12 OCT 17 STN(R) AnaVist(TM), Version 1.01, allows the export/download
                of CAplus documents for use in third-party analysis and
                visualization tools
NEWS 13 OCT 27 Free KWIC format extended in full-text databases
NEWS 14 OCT 27 DIOGENES content streamlined
NEWS 15 OCT 27 EPFULL enhanced with additional content
NEWS 16 NOV 14 CA/Caplus - Expanded coverage of German academic research
```

NEWS EXPRESS JUNE 13 CURRENT WINDOWS VERSION IS V8.0, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 13 JUNE 2005

NEWS	HOURS	STN Operating Hours Plus Help Desk Availability
NEWS	INTER	General Internet Information
NEWS	LOGIN	Welcome Banner and News Items
NEWS	PHONE	Direct Dial and Telecommunication Network Access to STN
NEWS	WWW	CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

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FILE 'HOME' ENTERED AT 10:20:26 ON 17 NOV 2005

=>

Uploading

THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE Do you want to switch to the Registry File?

Choice (Y/n):

Switching to the Registry File...

Some commands only work in certain files. For example, the EXPAND command can only be used to look at the index in a file which has an index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of commands which can be used in this file.

=> FILE REGISTRY

COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.21 0.21

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 10:20:38 ON 17 NOV 2005 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 15 NOV 2005 HIGHEST RN 868125-94-4 DICTIONARY FILE UPDATES: 15 NOV 2005 HIGHEST RN 868125-94-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

* The CA roles and document type information have been removed from * the IDE default display format and the ED field has been added, *

* effective March 20, 2005. A new display format, IDERL, is now

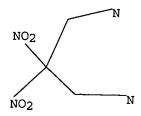
Structure search iteration limits have been increased. See HELP SLIMITS for details.

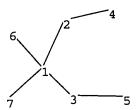
REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>

Uploading C:\Program Files\Stnexp\Queries\10604774.str





chain nodes :

1 2 3 4 5 6 7

chain bonds :

1-2 1-3 1-6 1-7 2-4 3-5

exact/norm bonds :

2-4 3-5 exact bonds : 1-2 1-3 1-6 1-7

Match level :

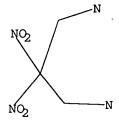
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS

L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 11

SAMPLE SEARCH INITIATED 10:20:52 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 11 TO ITERATE

100.0% PROCESSED 11 ITERATIONS 5 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
PROJECTED ITERATIONS: 22 TO 418
PROJECTED ANSWERS: 5 TO 234

L2 5 SEA SSS SAM L1

10604774.trn Page 3 10:44

=> s l1 sss full

FULL SEARCH INITIATED 10:20:59 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 185 TO ITERATE

65 ANSWERS

100.0% PROCESSED 185 ITERATIONS

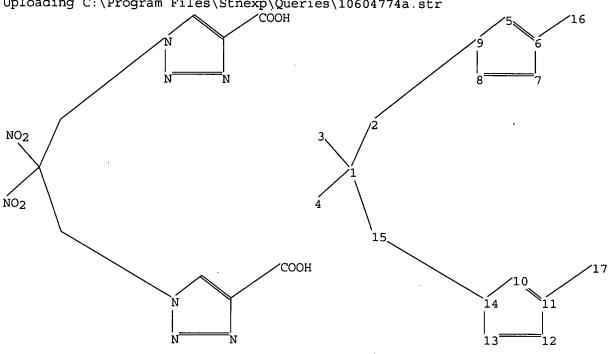
SEARCH TIME: 00.00.01

65 SEA SSS FUL L1

=>

L3

Uploading C:\Program Files\Stnexp\Queries\10604774a.str



chain nodes :

1 2 3 4 15 16 17

ring nodes :

 $5\quad \bar{6}\quad 7\quad 8\quad 9\quad 10\quad 11\quad 12\quad 13\quad 14$

chain bonds :

1-2 1-4 1-3 1-15 2-9 6-16 11-17 14-15

ring bonds :

5-6 5-9 6-7 7-8 8-9 10-11 10-14 11-12 12-13 13-14

exact/norm bonds :

2-9 5-9 6-7 7-8 8-9 10-14 11-12 12-13 13-14 14-15

exact bonds :

1-2 1-4 1-3 1-15 5-6 6-16 10-11 11-17

isolated ring systems :

containing 5 : 10 :

Match level :

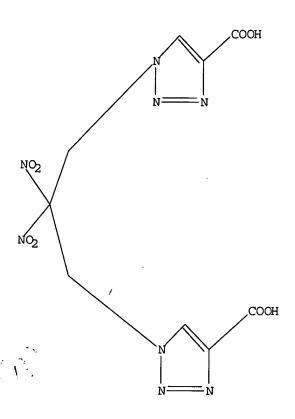
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:CLASS 16:CLASS 17:CLASS

L4 STRUCTURE UPLOADED

=> d 14

L4 HAS NO ANSWERS

L4 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 14

SAMPLE SEARCH INITIATED 10:28:12 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 0 TO ITERATE

100.0% PROCESSED

0 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS:

0 TO

PROJECTED ANSWERS:

TO 0

L5

0 SEA SSS SAM L4

=> s l4 sss full

FULL SEARCH INITIATED 10:28:18 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED -

3 TO ITERATE

0

100.0% PROCESSED

3 ITERATIONS

SEARCH TIME: 00.00.01

1 ANSWERS

10604774.trn

Page 5

L6 1 SEA SSS FUL L4

=>

chain nodes : 1 2 3 14 15 16 18 24 ring nodes : 4 5 6 7 8 9 10 11 12 13 19 20 21 22 23 chain bonds : 1-2 1-14 1-3 1-18 2-8 5-15 10-16 13-14 18-20 23-24 ring bonds : 4-5 4-8 5-6 6-7 7-8 9-10 9-13 10-11 11-12 12-13 19-20 19-23 20-21 21-22 22-23 exact/norm bonds : 1-3 2-8 4-8 5-6 6-7 7-8 9-13 10-11 11-12 12-13 13-14 18-20 19-20 20-21 21-22 22-23 exact bonds : 1-2 1-14 1-18 4-5 5-15 9-10 10-16 19-23 23-24 isolated ring systems : containing 4 : 9 : 19 :

Match level :

1:CLASS 2:CLASS 3:CLASS 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS 16:CLASS 18:CLASS 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:CLASS

10:44

L7 STRUCTURE UPLOADED

=> d 17 L7 HAS NO ANSWERS

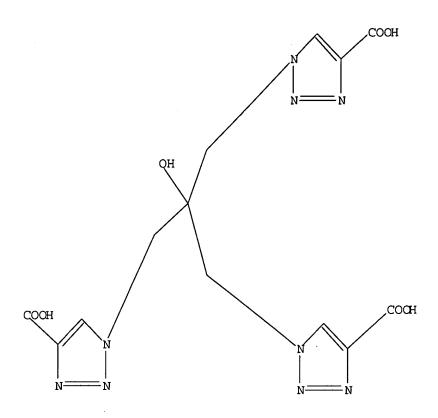
10604774.trn Page 6

11/17/2005

10604774.trn

L7

STR



Structure attributes must be viewed using STN Express query preparation.

=> s 17

SAMPLE SEARCH INITIATED 10:32:57 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 0 TO ITERATE

100.0% PROCESSED

0 ITERATIONS

0 ANSWERS

1 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:

ONLINE **COMPLETE**

BATCH

COMPLETE

PROJECTED ITERATIONS:

0 TO

PROJECTED ANSWERS:

0 TO

L8

0 SEA SSS SAM L7

=> s 17 sss full

FULL SEARCH INITIATED 10:33:04 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED -

21 TO ITERATE

100.0% PROCESSED

21 ITERATIONS

SEARCH TIME: 00.00.01

1 SEA SSS FUL L7

L9

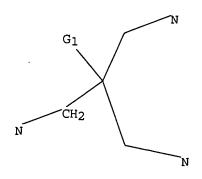
1 3EA 333 FUL L/

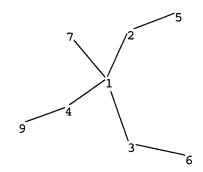
=>

Uploading C:\Program Files\Stnexp\Queries\10604774c.str

10604774.trn

Page 7





chain nodes :

1 2 3 4 5 6 7 9

chain bonds :

1-2 1-3 1-4 1-7 2-5 3-6 4-9

exact/norm bonds : 1-7 2-5 3-6 exact bonds : 1-2 1-3 1-4 4-9

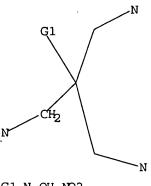
G1:N,OH,NO2

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 9:CLASS

L10 STRUCTURE UPLOADED

=> d 110 L10 HAS NO ANSWERS L10 STR



G1 N,OH,NO2

Structure attributes must be viewed using STN Express query preparation.

=> s 110 SAMPLE SEARCH INITIATED 10:37:18 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 1721 TO ITERATE

10604774.trn

Page 8

100.0% PROCESSED 1721 ITERATIONS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS:

31932 TO 36908

PROJECTED ANSWERS:

2 TO 124

L11

2 SEA SSS SAM L10

=> s 110 sss full

FULL SEARCH INITIATED 10:37:24 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 33969 TO ITERATE

100.0% PROCESSED 33969 ITERATIONS

SEARCH TIME: 00.00.01

.12 24 SEA SSS FUL L10

=> FIL HCAPLUS

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

2 ANSWERS

FULL ESTIMATED COST

ENTRY SESSION

655.64 655.85

FILE 'HCAPLUS' ENTERED AT 10:37:31 ON 17 NOV 2005
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FILE COVERS 1907 - 17 Nov 2005 VOL 143 ISS 21 FILE LAST UPDATED: 16 Nov 2005 (20051116/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d his

(FILE 'HOME' ENTERED AT 10:20:26 ON 17 NOV 2005)

FILE 'REGISTRY' ENTERED AT 10:20:38 ON 17 NOV 2005

L1 STRUCTURE UPLOADED

L2 5 S L1

L3 65 S L1 SSS FULL

L4 STRUCTURE UPLOADED

L5 0 S L4

10604774.trn

Page 9

```
11/17/2005 10604774.trn
L6
              1 S L4 SSS FULL
L7
               STRUCTURE UPLOADED
L8
              0 S L7
L9
              1 S L7 SSS FULL
L10
                STRUCTURE UPLOADED
L11
              2 S L10
L12
             24 S L10 SSS FULL
     FILE 'HCAPLUS' ENTERED AT 10:37:31 ON 17 NOV 2005
=> s 13
            47 L3 (
L13
=> s 113 and polyazido
            18 POLYAZIDO
             2 L13 AND POLYAZIDO
L14
 => s 113 and azide
         40607 AZIDE
          8478 AZIDES
         42978 AZIDE
                  (AZIDE OR AZIDES)
L15
             8 L13 AND AZIDE
=> s 113 and py<=2002
      22790379 PY<=2002
L16
            41 L13 AND PY<=2002
=> s 16
L17
             2 L6
=> s 19
L18
                                                  Mulas
=> s 112
            20 L12
=> s 119 and polyazido
            18 POLYAZIDO
L20
             3 L19 AND POLYAZIDO
=> d l14 ibib abs hitstr tot
L14 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER:
                         2005:29032 HEAPLUS
DOCUMENT NUMBER:
                         142:114074
TITLE:
                         Preparation of polyazido carboxylic acid
                         esters
INVENTOR(S):
                         Dave, Paritosh R.; Duddu, Raja G.; Damavarapu, Reddy;
                         Gelber, Nathaniel; Yang, Kathy; Surapaneni, C. Rao
PATENT ASSIGNEE(S):
                         United States Dept. of the Army, USA
SOURCE:
                         U.S., 9 pp.
                         CODEN: USXXAM
DOCUMENT TYPE:
                         Patent
LANGUAGE:
                         English
FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:
     PATENT NO.
                         KIND DATE
                                           APPLICATION NO.
                                                                   DATE
```

10:44

10604774.trn

Page 10

Y X
$$Z$$
 HO_2C N N N N CO_2H CO_2

AB This invention relates to a series of novel compds., such as I = N3, OH, ONO2, NO2; Y = CH2N3, NO2; A, B = N3, 4-carboxytriazolomethyl], and II [Z = CH2, O, NOH, 2,4-dihydrophenylhydrozono], including 2-azido-2-azidomethyl-1,3-diazidopropane, 2-azidomethyl-2-hydroxy-1,3diazidopropane, 2-azidomethyl-2-nitrato-1,3-diazidopropane, 2-azidomethyl-2-nitro-1,3-diazidopropane, 2,2-dinitro-1,3-diazidopropane, methallyidiazide, a dimer of methallyidiazide, comprising 3a,8a-bis-azidomethyl-3a,4,8a,9-tetrahydro-3H,8H-bis[1,2,3]triazolo[1,5-a; 1'',5''-d]pyrazine, 1,3-diazidoacetone, and 2-oximido-1,3-diazidopropane. Also shown are reaction intermediates of these compds., including 2,2-bis(chloromethyl)oxirane, and 2,2-bis(azidomethyl)oxirane. In addition, a number of potentially useful energetic compds. have been prepared from the low mol. weight polyazido compds. above, including N-2(azido-1-azidomethyl-ethylidene)-N''-(2,4-dinitrophenyl)-hydrazine (7-DNPH), 1,3-bis(4-carboxytriazolyl)2,2-dinitropropane, tris(4-carboxytriazolomethyl)methanol, benzene-1,3,5-tricarboxylic acid tris(2-azido-1,1-bisazidomethyl-ethyl)ester, adamantane 1,3,5,7-tetracarboxylic acid tetrakis(2-azido-1,1-bisazidomethylethyl)ester, adamantane carboxylic acid (2-azido-1,1-bisazidomethylethyl)ester, cubane 1,3,5,7-tetracarboxylic acid tetrakis (2-azido-1,1-bisazidomethyl-ethyl)ester, cubane 1,4-dicarboxylic acid bis(2-azido-1,1-bisazidomethyl-ethyl)ester. Thus, tris(4carboxytriazolomethyl) methanol (III) was prepared by the reaction of 2-azidomethyl-2-hydroxy-1,3-diazidopropane I [A, B = N3; X = CH2N3; Y = OH] (also prepared) with propiolic acid. IT 682353-68-0P, 2,2-Dinitro-1,3-diazidopropane RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of polyazido carboxylic acid esters derived from methallyl dichloride) RN

RN 682353-68-0 HCAPLUS CN Propane, 1,3-diazido-2,2-dinitro- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE/6 CITED REFERENCES AVAILABLE FOR THIS 6 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 2 OF 2 HCAPLUS COPYRIGHT/2005 ACS on STN

ACCESSION NUMBER:

2004:137939 /HCAPLUS

DOCUMENT NUMBER:

140:357709

TITLE:

Preparation of cage molecule based polyazido

core units for dendrimer synthesis

AUTHOR (S): Dave, Paritosh R.; Duddu, Raja; Yang, Kathy;

Damavarapu, Reddy; Gelber, Nathaniel; Surapaneni, Rao;

Gilardi, Richard

CORPORATE SOURCE:

GEO-CENTERS, INC. at ARDEC, Picatinny Arsenal, NJ,

07806-5000, USA

SOURCE:

Tetrahedron Letters (2004), 45(10), 2159-2162

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER:

Elsevier Science B.V.

DOCUMENT TYPE:

Journal

LANGUAGE:

English

Core mols. based on benzene-, cubane-, and adamantane-polycarboxylates with peripheral polyazido substitution were prepared The first synthesis of 1,3-diazidoacetone and its conversion to the corresponding oxime, DNPH, and 2,2-dinitro derivs. is also reported. All azido compos. should be considered dangerous and proper precautions should be taken during handling and storage of these mols.

IT 682353-68-0P

> RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of peripheral polyazido and benzene and cubane and adamantane core unit cages for triazole and tetrazole containing dendrimer synthesis)

RN 682353-68-0 HCAPLUS

CN Propane, 1,3-diazido-2,2-dinitro- (9CI) (CA INDEX NAME)

$$NO_{2}$$
 $N_{3}-CH_{2}-C-CH_{2}-N_{3}$
 NO_{2}

REFERENCE COUNT:

17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d l15 ibib abs hitstr tot

L15 ANSWER 1 OF 8 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

2005:29032 HCAPLUS

DOCUMENT NUMBER:

142:114074

TITLE: INVENTOR (S):

Preparation of polyazido carboxylic acid esters Dave, Paritosh R.; Duddu, Raja G.; Damavarapu, Reddy; Gelber, Nathaniel; Yang, Kathy; Surapaneni, C. Rao

"United States Dept. of the Army, USA

PATENT ASSIGNEE(S): SOURCE: "U"S., 9 pp.

CODEN: USXXAM

DOCUMENT TYPE:

Patent

LANGUAGE:

English

10604774.trn

Page 12

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6841690	B1	20050111	US 2003-604778	20030815
US 6965042	B1	20051115	US 2003-604777	20030815
PRIORITY APPLN. INFO.:			US 2002-319801P	P 20021219
CI				

Y X
$$Z$$
 HO_2C N N N N CO_2H CO_2

AB This invention relates to a series of novel compds., such as I [X = N3]OH, ONO2, NO2; Y = CH2N3, NO2; A, B = N3, 4-carboxytriazolomethyll, and II [Z = CH2, O, NOH, 2,4-dihydrophenylhydrozono], including 2-azido-2-azidomethyl-1,3-diazidopropane, 2-azidomethyl-2-hydroxy-1,3diazidopropane, 2-azidomethyl-2-nitrato-1,3-diazidopropane, 2-azidomethyl-2-nitro-1,3-diazidopropane, 2,2-dinitro-1,3-diazidopropane, methallyidiazide, a dimer of methallyidiazide, comprising 3a,8a-bis-azidomethyl-3a,4,8a,9-tetrahydro-3H,8H-bis[1,2,3]triazolo[1,5-a; 1'',5''-d]pyrazine, 1,3-diazidoacetone, and 2-oximido-1,3-diazidopropane. Also shown are reaction intermediates of these compds., including 2,2-bis(chloromethyl)oxirane, and 2,2-bis(azidomethyl)oxirane. In addition, a number of potentially useful energetic compds. have been prepared from the low mol. weight polyazido compds. above, including N-2(azido-1-azidomethylethylidene) -N''-(2,4-dinitrophenyl) -hydrazine (7-DNPH), 1,3-bis(4-carboxytriazolyl)2,2-dinitropropane, tris(4carboxytriazolomethyl) methanol, benzene-1,3,5-tricarboxylic acid tris(2-azido-1,1-bisazidomethyl-ethyl)ester, adamantane 1,3,5,7-tetracarboxylic acid tetrakis(2-azido-1,1-bisazidomethylethyl)ester, adamantane carboxylic acid (2-azido-1,1-bisazidomethylethyl)ester, cubane 1,3,5,7-tetracarboxylic acid tetrakis (2-azido-1,1-bisazidomethyl-ethyl)ester, cubane 1,4-dicarboxylic acid bis(2-azido-1,1-bisazidomethyl-ethyl)ester. Thus, tris(4carboxytriazolomethyl)methanol (III) was prepared by the reaction of 2-azidomethyl-2-hydroxy-1,3-diazidopropane I [A, B = N3; X = CH2N3; Y = OH] (also prepared) with propiolic acid. IT **682353-68-0P**, 2,2-Dinitro-1,3-diazidopropane RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic

preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of polyazido carboxylic acid esters derived from methallyl dichloride)

RN 682353-68-0 HCAPLUS

CN Propane, 1,3-diazido-2,2-dinitro- (9CI) (CA INDEX NAME)

$$N_3 - CH_2 - C - CH_2 - N_3$$
 N_{O_2}

REFERENCE COUNT:

THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 2 OF 8 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:137939 HCAPLUS

DOCUMENT NUMBER: 140:357709

TITLE:

AUTHOR (S):

Preparation of cage molecule based polyazido core

units for dendrimer synthesis

Dave, Paritosh R.; Duddu, Raja; Yang, Kathy;

Damawarapu, Reddy; Gelber, Nathaniel; Surapaneni, Rao;

Gilardi, Richard

CORPORATE SOURCE: GEO-CENTERS, INC. at ARDEC, Picatinny Arsenal, NJ,

07806-5000, USA

SOURCE: Tetrahedron Letters (2004), 45(10), 2159-2162

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal LANGUAGE: English

AB Core mols. based on benzene-, cubane-, and adamantane-polycarboxylates with peripheral polyazido substitution were prepared. The first synthesis of 1,3-diazidoacetone and its conversion to the corresponding oxime, DNPH, and 2,2-dinitro derivs. is also reported. All azido compds. should be considered dangerous and proper precautions should be taken during handling and storage of these mols.

IT 682353-68-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of peripheral polyazido and benzene and cubane and adamantane core unit cages for triazole and tetrazole containing dendrimer synthesis)

RN 682353-68-0 HCAPLUS

CN Propane, 1,3-diazido-2,2-dinitro- (9CI) (CA INDEX NAME)

$$N_3 - CH_2 - C - CH_2 - N_3$$
 $N_3 - CH_2 - N_3$
 N_{O_2}

REFERENCE COUNT:

17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 3 OF 8 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1998:666542 HCAPLUS

DOCUMENT NUMBER:

130:15525

TITLE:

Thermal decomposition of organic azides in

propellants

AUTHOR(S):

Jin, Shaohua; Li, Wen; Song, Quancai

CORPORATE SOURCE:

College of Chemical Engineering and Materials, Beijing

10604774.trn

Page 14

Institute of Technology, Beijing, 100081, Peop. Rep.

China

SOURCE: Hanneng Cailiao (1998), 6(3), 123-127

CODEN: HACAFQ; ISSN: 1006-9941

PUBLISHER: Hanneng Cailiao Bianjibu

DOCUMENT TYPE: Journal LANGUAGE: Chinese

AB The thermal decomposition of 11 compds. containing azidomethyl-gem-dinitro groups

was studied by DTA, and the formal kinetic parameters E and A were obtained. Comparison of the kinetic parameters of some azides with those of trinitromethyl compds. with structures similar to the corresponding compds. shows that E values increase due to the introduction of azide-group. The influences of the number and position of azidomethyl-gem-dinitro groups on the thermal decomposition kinetic parameters of azidomethyl derivs. were also studied.

IT 169564-63-0 169564-64-1 180842-20-0

RL: PRP (Properties); TEM (Technical or engineered material use); USES (Uses)

(thermal decomposition of organic azides in propellants)

RN 169564-63-0 HCAPLUS

CN 1,2-Ethanediamine, N,N'-bis(3-azido-2,2-dinitropropyl)-N,N'-dinitro- (9CI) (CA INDEX NAME)

RN 169564-64-1 HCAPLUS

CN 1-Propanamine, 3-azido-N-methyl-N,2,2-trinitro- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{NO}_2 & \text{NO}_2 \\ & & \\ \text{Me} - \text{N} - \text{CH}_2 - \text{C} - \text{CH}_2 - \text{N}_3 \\ & & \\ & \text{NO}_2 \end{array}$$

RN 180842-20-0 HCAPLUS

CN 1-Propanamine, 3-azido-N-(3-azido-2,2-dinitropropyl)-N,2,2-trinitro- (9CI) (CA INDEX NAME)

L15 ANSWER 4 OF 8 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1997:415029 HCAPLUS

DOCUMENT NUMBER: 127:95011

10604774.trn

Page 15

TITLE: Synthesis of 3-azido-2,2-dinitropropyl-substituted

nitramines

AUTHOR(S): Yan, Hong; Guan, Xiao-Pei

CORPORATE SOURCE: Dep. Chem. and Environmental Engineering, Beijing

Polytechnic Univ., Beijing, 100022, Peop. Rep. China

SOURCE: Youji Huaxue (1997), 17(3), 284-288

CODEN: YCHHDX; ISSN: 0253-2786

PUBLISHER: Kexue

DOCUMENT TYPE: Journal LANGUAGE: Chinese

AB Title azides MeN(NO2)CH2C(NO2)2CH2N3,

[CH2N(NO2)CH2C(NO2)2CH2N3]2, and O2NN[CH2C(NO2)2CH2N3]2 were prepared from

alcs. MeN(NO2)CH2C(NO2)2CH2OH, [CH2N(NO2)CH2C(NO2)2CH2OH]2, and

O2NN[CH2C(NO2)2CH2OH]2 via the corresponding triflats.

IT 169564-63-0P 169564-64-1P 180842-20-0P

RL: SPN (Synthetic preparation); PREP (Preparation)

(synthesis of 3-azido-2,2-dinitropropyl-substituted nitramines)

RN 169564-63-0 HCAPLUS

CN 1,2-Ethanediamine, N,N'-bis(3-azido-2,2-dinitropropyl)-N,N'-dinitro- (9CI) (CA INDEX NAME)

RN 169564-64-1 HCAPLUS

CN 1-Propanamine, 3-azido-N-methyl-N,2,2-trinitro- (9CI) (CA INDEX NAME)

$$NO_2$$
 NO_2 NO_2 NO_2 NO_2 NO_2 NO_2 NO_2

RN 180842-20-0 HCAPLUS

CN 1-Propanamine, 3-azido-N-(3-azido-2,2-dinitropropyl)-N,2,2-trinitro- (9CI) (CA INDEX NAME)

L15 ANSWER 5 OF 8 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1996:514610 HCAPLUS

DOCUMENT NUMBER: 125:172480

TITLE: Synthesis of high density azidonitramines AUTHOR(S): Yan, Hong; Guan, Xiao-Pei; Chen, Bo-Ren

CORPORATE SOURCE: Dep. of Chemistry and Environmental Engineering,

10604774.trn

Page 16

Beijing Polytechnic Univ., Beijing, 100022, Peop. Rep.

China

SOURCE: International Annual Conference of ICT (1996),

27th (Energetic Materials), 135.1-135.5

CODEN: IACIEQ

PUBLISHER: Fraunhofer-Institut fuer Chemische Technologie

DOCUMENT TYPE: Journal LANGUAGE: English

AB Three nitramines containing the 2-azido-1,1-dinitroethyl group have been synthesized, one of which, 1,7-diazido-2,2,4,6,6-pentanitro-4-azaheptane, possesses a d. of 1.835 g/cm3. For these compds. the mol. structures have been determined, and some of the properties (e.g., decomposition point) are also

reported.

IT 169564-63-0P 169564-64-1P 180842-20-0P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and properties of)

RN 169564-63-0 HCAPLUS

CN 1,2-Ethanediamine, N,N'-bis(3-azido-2,2-dinitropropyl)-N,N'-dinitro- (9CI) (CA INDEX NAME)

RN 169564-64-1 HCAPLUS

CN 1-Propanamine, 3-azido-N-methyl-N,2,2-trinitro- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{NO}_2 & \text{NO}_2 \\ & & & \\ \text{Me-N-CH}_2 - \text{C-CH}_2 - \text{N}_3 \\ & & \\ & & \text{NO}_2 \end{array}$$

RN 180842-20-0 HCAPLUS

CN 1-Propanamine, 3-azido-N-(3-azido-2,2-dinitropropyl)-N,2,2-trinitro- (9CI) (CA INDEX NAME)

L15 ANSWER 6 OF 8 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1995:830797 HCAPLUS

DOCUMENT NUMBER: 123:291159

TITLE: Development of energetic additives for propellants in

China

AUTHOR(S): Ou, Yuxiang; Chen, Boren; Yan, Hong; Jia, Huiping; Li,

10604774.trn Page 17 10:44

Jianjun; Dong, Shuan

CORPORATE SOURCE: Department Chemical Engineering, Beijing Institute

Technology, Beijing, 100081, Peop. Rep. China

SOURCE: Journal of Propulsion and Power (1995), 11(4), 838-47

CODEN: JPPOEL; ISSN: 0748-4658

PUBLISHER: American Institute of Aeronautics and Astronautics

DOCUMENT TYPE: Journal LANGUAGE: English

The development of energetic azide binders and plasticizers for solid propellants in China was described, focusing on 14 azides. The reaction routes and conditions for preparing these azides were summarized; the performance of the azides, including d., m.p.,

enthalpy of formation, thermal decomposition temperature (determined by differential

scanning calorimetry or DTA), impact sensitivity, etc, were presented. The azides were arranged in six categories: (1) azide polyethers (glycidyl azide polymer, 3,3-bis(azidomethyl)oxetane (BAMO) homopolymer, and BAMO-tetrahydrofuran copolymer), (2) azidonitramines (1,5-diazido-3-nitrazapentane, N-nitro-N-azidomethyl-gemdinitroethylmethylamine, and N,N'-bis(azidomethyl-gemdinitroethyl)ethylenedinitramine), (3) azidonitro compds. [2-nitro-2-methyl-1,3-diazidopropane, 2-nitro-2-azidomethyl-1,3diazidopropane, and 1-azido-2-(2,4,6-trinitrophenyl)ethane], (4) aliphatic azides (1,2,4,triazidobutane and tetraazidomethylemethane), (5) azidonitrates (pentaerythritol diazidodinitrate), and (6) oxygen heterocyclic azides (3-azidomethyl-3-ethyloxetane and 2,2-dimethyl-5-azidomethyl-5-nitro-1,3-dioxane).

ΙT 169564-63-0P 169564-64-1P

> RL: IMF (Industrial manufacture); NUU (Other use, unclassified); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); USES (Uses) (development, synthesis, and properties of energetic binders and plasticizers for solid propellants)

RN169564-63-0 HCAPLUS

CN 1,2-Ethanediamine, N,N'-bis(3-azido-2,2-dinitropropyl)-N,N'-dinitro- (9CI) (CA INDEX NAME)

169564-64-1 HCAPLUS

CN 1-Propanamine, 3-azido-N-methyl-N,2,2-trinitro- (9CI) (CA INDEX NAME)

L15 ANSWER 7 OF 8 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1967:453645 HCAPLUS

DOCUMENT NUMBER: 67:53645

10604774.trn Page 18

TITLE: Preparation of nitro aza diisocyanates suitable as

explosives

INVENTOR(S): Vanneman, Clinton R.; Klager, Karl

PATENT ASSIGNEE(S): Aerojet-General Corp.

SOURCE: Ger., 3 pp. CODEN: GWXXAW

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

	PATENT NO.	KIND	DATE	APPLICATION	NO.	DATE
		-				
	DE 1238901		19670420	DE		19601201
AB	An outline of the	synthesi	s of the tit	le compds. (I) is given	. Nitro az
	dicarboxylic acids	(TT) we	re prepared	either by by	drolveis of	the

Α za dicarboxylic acids (II) were prepared either by hydrolysis of the corresponding nitro aza dinitriles or by condensation of a nitro diol with an amino ester, followed by HNO3 oxidation The various II were converted to the corresponding acid chlorides (III) with SOCl2. Treatment of III with NaN3, KN3, or Mg(N3)2 at 0-5° gave the corresponding azides , which were converted to I by a Curtius rearrangement. Thus, a solution of 11 g. 4,7,7,10-tetranitro-4,10-diaza-1,13-tridecanedicarbonyl chloride in 50 ml. Me2CO was added dropwise to a solution of 4.6 q. NaN3 in 15 ml. H2O (kept at 5°). The mixture was stirred 1 hr. at 0° and filtered. The residue was washed with H2O and (CH2Cl2)2 and dried in vacuo to give 3,6,6,9-tetranitro-3,9-diazaundecamethylene diisocyanate, m. 88-90° (CHC13).

IT 17695-19-1

> RL: RCT (Reactant); RACT (Reactant or reagent) (explosive properties of)

RN 17695-19-1 HCAPLUS

CNIsocyanic acid, (2,2-dinitrotrimethylene)bis[(nitroimino)methylene] ester (8CI) (CA INDEX NAME)

L15 ANSWER 8 OF 8 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1963:461451 HCAPLUS

DOCUMENT NUMBER: 59:61451 ORIGINAL REFERENCE NO.: 59:11236b-g

TITLE: Synthesis and reactions of trinitromethyl compounds

AUTHOR(S): Frankel, M. B.

CORPORATE SOURCE: Stanford Res. Inst., Menlo Park, CA SOURCE: Tetrahedron (1963), 19(Suppl. 1), 213-17

CODEN: TETRAB; ISSN: 0040-4020

DOCUMENT TYPE: Journal LANGUAGE: Unavailable

A systematic study of the synthesis of trinitromethyl compds. from HC(NO2)3 and (O2N)3CCH2OH (I) is summarized. HC(NO2)3 adds readily in a Michael type of addition to α, β -unsatd. compds. such as H2C:CHCO2H and its esters, HOCH2COCH:CH2, and O2NCH:CH2 to yield 83% (NO2) 3CCH2CH2CO2H, m. 61°; 64% (NO2) 3CCH2CH2CO2CH: CH2, b6

from

85-9°, n25D 1.4707; 71% (NO2)3CCH2CH2CO2CH2- CH:CH2, b0.3 71-2°, n25D 1.4676; 74% (NO2)3CCH2CH2CO- CH2OH, m. 77°; and 50% (NO2)3CCH2CH2NO2, m. 50-1°. Of special interest was addition of HC(NO2)3 to H2C:C(NO2)CH2OAc (II). Condensation of MeNO2 with HCHO in the presence of NaOH gave the acid Na salt, HOCH2C(: NO2Na)CH2OH, which was acidified and acetylated to give AcOCH2CH(NO2)CH2OAc, and converted by vapor phase cleavage at 180°/100 mm. to II. Addition of MeCH(NO2)2 to II gave MeC(NO2)2CH2CH(NO2)CH2C(NO2)2Me, and in similar manner, addition of HC(NO2)3 to II yielded (NO2)3CCH2CH(NO2)CH2C(NO2)3. It was of interest to determine the various types of trinitromethyl compds. that could be prepared

(NO2)3CCH2CH2CO2H (III). III refluxed 4 hrs. with SOCl2 yielded 33% [(NO2)3CCH2CH2CO]2O, m. 109-10°, but 20 hrs. refluxing gave 82% (NO2)3CCH2CH2COCl (IV), b0.5 65-6°, n25D 1.4835. IV treated with NaN3 gave the azide, converted in situ to 71.2% (NO2)3CCH2CH2NCO (V), b10 73-5°, n25D 1.4805. V hydrolyzed with HCl yielded 94% (NO2)3CCH2CH2NH2.HCl (VI), m. 161-3°. V and VI were used for the preparation of trinitromethyl carbamates (VII) and trinitromethylamines (VIII). VII were prepared by addition of I to various isocyanates and the addition of different alcs. to V. I is considerably more acidic than ordinary alcs. and reacts less readily with isocyanates. I refluxed with an isocyanate in CHCl3 several hrs. in the presence of a catalytic amount of ferric acetonylacetonate gave essentially quant. yields of the tabulated VII. All were nitrated to the corresponding N-nitro derivs. VIII were prepared by the Mannich condensation of I with various primary amines and the reaction of VI with nitro alcs. Since nitro alcs. are demethylolated in the presence of base, the condensations were carried out by portionwise addition

precipitation of the tabulated VIII. All these secondary amines were nitrated to the corresponding nitramines. The reaction of (HOCH2)2C(NO2)2 with VI and HCHO yielded 40.8% 1,3-bis-(3,3,3-trinitropropyl)-5,5dinitroperhydropyrimidine, m. 119-21°. Condensation of VI with HCHO gave a quant. yield of 1,3,5-tris(3,3,3-trinitropropyl)perhydro-1,3,5triazine, m. 121-3°. Esters of I were prepared according to the procedure of Hill (CA 49, 8103f) by treating the acid chlorides with I in the presence of a catalytic amount of AlCl3. The esterification of 4,4,6,6,8,8-hexanitroundecanedioic acid was carried out in 100% H2SO4 as the ionizing solvent. The 2,2,2-trinitroethyl esters prepared are summarized (ester, % yield, and m.p. given): N(NO2)[CH2CO2CH2C(NO2)3]2, 77.8, 160.0-60.5°; N(NO2) [CH2CH2CO2CH2C(NO2)3]2, 35.9, 110-11°; [CH2N(NO2) CH2CO2CH2C(NO2) 3] 2, 5.6, 195-7°; [CH2N(NO2)CH2CH2CO2CH2C(NO2)3]2 85.5, 126-8°; MeC(NO2)2CH2N(NO2)CH2CO2CH2C(NO2)3, 50.3, 121.0-1.5°; C(NO2)2[CH2CH2CO2CH2C(NO2)3]2, 47.0, 170-1°; C-(NO2)2[CH2C(NO2)2CH2CH2CO2CH2C(NO2)3]2, 87.8, 117-18°.

of an equivalent amount of base to VI and nitro alc. in H2O with immediate

RN 49614-89-3 HCAPLUS

OH, ONO2, NO2; Y = CH2N3, NO2; A, B = N3, 4-carboxytriazolomethyl], and II [Z = CH2, O, NOH, 2,4-dihydrophenylhydrozono], including 2-azido-2-azidomethyl-1,3-diazidopropane, 2-azidomethyl-2-hydroxy-1,3diazidopropane, 2-azidomethyl-2-nitrato-1,3-diazidopropane, 2-azidomethyl-2-nitro-1,3-diazidopropane, 2,2-dinitro-1,3-diazidopropane, methallyidiazide, a dimer of methallyidiazide, comprising 3a,8a-bis-azidomethyl-3a,4,8a,9-tetrahydro-3H,8H-bis[1,2,3]triazolo[1,5-a; 1'',5''-d]pyrazine, 1,3-diazidoacetone, and 2-oximido-1,3-diazidopropane. Also shown are reaction intermediates of these compds., including 2,2-bis(chloromethyl)oxirane, and 2,2-bis(azidomethyl)oxirane. In addition, a number of potentially useful energetic compds. have been prepared from the low mol. weight polyazido compds. above, including N-2(azido-1-azidomethylethylidene) -N''-(2,4-dinitrophenyl) -hydrazine (7-DNPH), 1,3-bis(4-carboxytriazolyl)2,2-dinitropropane, tris(4carboxytriazolomethyl)methanol, benzene-1,3,5-tricarboxylic acid tris(2-azido-1,1-bisazidomethyl-ethyl)ester, adamantane 1,3,5,7-tetracarboxylic acid tetrakis(2-azido-1,1-bisazidomethylethyl)ester, adamantane carboxylic acid (2-azido-1,1-bisazidomethylethyl)ester, cubane 1,3,5,7-tetracarboxylic acid tetrakis (2-azido-1,1-bisazidomethyl-ethyl)ester, cubane 1,4-dicarboxylic acid bis(2-azido-1,1-bisazidomethyl-ethyl)ester. Thus, tris(4carboxytriazolomethyl) methanol (III) was prepared by the reaction of 2-azidomethyl-2-hydroxy-1,3-diazidopropane I [A, B = N3; X = CH2N3; Y = OH] (also prepared) with propiolic acid.

IT 682353-70-4P

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(preparation of polyazido carboxylic acid esters derived from methallyl dichloride)

RN 682353-70-4 HCAPLUS

CN 1H-1,2,3-Triazole-4-carboxylic acid, 1,1'-(2,2-dinitro-1,3-propanediyl)bis-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & &$$

REFERENCE COUNT:

THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2005 ACS on STN

6

ACCESSION NUMBER:

2004:137939 HCAPLUS

DOCUMENT NUMBER:

140:357709

TITLE:

AUTHOR (S):

Preparation of eage molecule based polyazido core

whits for dendrimer synthesis

Pave, Paritosh R.; Duddu, Raja; Yang, Kathy;

Damavarapu, Reddy; Gelber, Nathaniel; Surapaneni, Rao;

Gilardi, Richard

CORPORATE SOURCE: GEO-CENTERS, INC. at ARDEC, Picatinny Arsenal, NJ,

07806-5000, USA

SOURCE: Tetrahed

Tetrahedron Letters (2004), 45(10), 2159-2162

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER:

Elsevier Science B.V.

10604774.trn

Page 22

RN 91004-98-7 HCAPLUS

CN 1,3-Propanediamine, 2,2-dinitro-N,N'-bis(3,3,3-trinitropropyl)- (6CI, 7CI) (CA INDEX NAME)

=> d l17 ibib abs hitstr tot

L17 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2005:29032 HCAPLUS

DOCUMENT NUMBER: 142:114074

TITLE:

Preparation of polyazido carboxylic acid esters Dave, Paritosh R.; Duddu, Raja G.; Damavarapu, Reddy; INVENTOR(S): Gelber, Nathaniel; Yang, Kathy; Surapaneni, C. Rao

winder

United States Dept. of the Army, USA PATENT ASSIGNEE(S):

SOURCE: U.S., 9 pp.

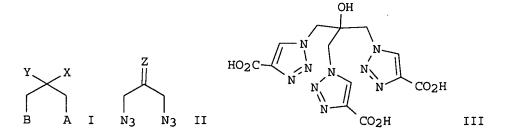
CODEN: USXXAM

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	API	PLICATION NO.		DATE
US 6841690	 В1	20059411	IIS	 2003-604778		20030815
US 6965042	B1	20051115		2003-604777		20030815
PRIORITY APPLN. INFO.:			US	2002-319801P	P	20021219



AB This invention relates to a series of novel compds., such as I = X = N3,

10604774.trn

Page 21

11/17/2005

10604774.trn

DOCUMENT TYPE:

Journal

LANGUAGE:

English

Core mols. based on benzene-, cubane-, and adamantane-polycarboxylates with peripheral polyazido substitution were prepared The first synthesis of 1,3-diazidoacetone and its conversion to the corresponding oxime, DNPH, and 2,2-dinitro derivs. is also reported. All azido compds. should be considered dangerous and proper precautions should be taken during handling and storage of these mols.

IT 682353-70-4P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of peripheral polyazido and benzene and cubane and adamantane core unit cages for triazole and tetrazole containing dendrimer synthesis)

682353-70-4 HCAPLUS RN

1H-1,2,3-Triazole-4-carboxylic acid, 1,1'-(2,2-dinitro-1,3-propanediyl)bis-CN (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & N & N - CH_2 - C - CH_2 - N & N \\ & NO_2 & & NO_2 & & CO_2H \end{array}$$

REFERENCE COUNT:

17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d l18 ibib abs hitstr tot

L18 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

2005:29032 HCAPLUS

DOCUMENT NUMBER: TITLE:

142:114074

INVENTOR (S):

Preparation of polyazido carboxylic acid esters

Dave, Paritosh R.; Duddu, Raja G.; Damavarapu, Reddy; Gelber, Nathanier; Yang, Kathy; Surapaneni, C. Rao

PATENT ASSIGNEE(S) United States Dept. of the Army, USA

SOURCE:

U.S., 9 pp. GODEN: USXXAM

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6841690	B1	20050111	US 2003-604778	20030815
OS_6965042/	B1	20051115	US 2003-604777	20030815
PRIORITY APPEN. INFO.:			US 2002-319801P I	20021219
GI				

Y X
$$Z$$
 HO_2C N N N N CO_2H CO_2

AB This invention relates to a series of novel compds., such as I [X = N3]OH, ONO2, NO2; Y = CH2N3, NO2; A, B = N3, 4-carboxytriazolomethyl], and II [Z = CH2, O, NOH, 2, 4-dihydrophenylhydrozono], including2-azido-2-azidomethyl-1,3-diazidopropane, 2-azidomethyl-2-hydroxy-1,3diazidopropane, 2-azidomethyl-2-nitrato-1,3-diazidopropane, 2-azidomethyl-2-nitro-1,3-diazidopropane, 2,2-dinitro-1,3-diazidopropane, methallyidiazide, a dimer of methallyidiazide, comprising 3a,8a-bis-azidomethyl-3a,4,8a,9-tetrahydro-3H,8H-bis[1,2,3]triazolo[1,5-a; 1'',5''-d]pyrazine, 1,3-diazidoacetone, and 2-oximido-1,3-diazidopropane. Also shown are reaction intermediates of these compds., including 2,2-bis(chloromethyl)oxirane, and 2,2-bis(azidomethyl)oxirane. In addition, a number of potentially useful energetic compds. have been prepared from the low mol. weight polyazido compds. above, including N-2(azido-1-azidomethylethylidene)-N''-(2,4-dinitrophenyl)-hydrazine (7-DNPH), 1,3-bis(4-carboxytriazolyl)2,2-dinitropropane, tris(4carboxytriazolomethyl)methanol, benzene-1,3,5-tricarboxylic acid tris(2-azido-1,1-bisazidomethyl-ethyl)ester, adamantane 1,3,5,7-tetracarboxylic acid tetrakis(2-azido-1,1-bisazidomethylethyl)ester, adamantane carboxylic acid (2-azido-1,1-bisazidomethylethyl)ester, cubane 1,3,5,7-tetracarboxylic acid tetrakis (2-azido-1,1-bisazidomethyl-ethyl)ester, cubane 1,4-dicarboxylic acid bis(2-azido-1,1-bisazidomethyl-ethyl)ester. Thus, tris(4carboxytriazolomethyl)methanol (III) was prepared by the reaction of 2-azidomethyl-2-hydroxy-1,3-diazidopropane I [A, B = N3; X = CH2N3; Y = OH] (also prepared) with propiolic acid.

IT 682353-71-5P, Tris(4-carboxytriazolomethyl)methanol
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP
(Preparation)

(preparation of polyazido carboxylic acid esters derived from methallyl dichloride)

RN 682353-71-5 HCAPLUS

CN 1H-1,2,3-Triazole-4-carboxylic acid, 1,1'-[2-[(4-carboxy-1H-1,2,3-triazol-1-yl)methyl]-2-hydroxy-1,3-propanediyl]bis- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

2004:137939 HCAPLUS

DOCUMENT NUMBER:

140:357709

TITLE:

Preparation of cage molecule based polyazido core

units for dendrimer synthesis

AUTHOR (S):

Dave, Paritosh K.; Duddu, Raja; Yang, Kathy;

Damavarapu, Reddy; Gelber, Nathaniel; Surapaneni, Rao; Gilardi, Richard

CORPORATE SOURCE:

GEO-CENTERS, INC. at ARDEC, Picatinny Arsenal, NJ,

-07806-5000, USA

SOURCE:

Tetrahedron Letters (2004), 45(10), 2159-2162

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER:

Elsevier Science B.V.

DOCUMENT TYPE:

LANGUAGE:

Journal English

AB Core mols. based on benzene-, cubane-, and adamantane-polycarboxylates with peripheral polyazido substitution were prepared The first synthesis of 1,3-diazidoacetone and its conversion to the corresponding oxime, DNPH, and 2,2-dinitro derivs. is also reported. All azido compds. should be considered dangerous and proper precautions should be taken during handling and storage of these mols.

IT 682353-71-5P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of peripheral polyazido and benzene and cubane and adamantane core unit cages for triazole and tetrazole containing dendrimer synthesis)

RN 682353-71-5 HCAPLUS

CN 1H-1,2,3-Triazole-4-carboxylic acid, 1,1'-[2-[(4-carboxy-1H-1,2,3-triazol-1-yl)methyl]-2-hydroxy-1,3-propanediyl]bis- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d l20 ibib abs hitstr tot

L20 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2005:29032 HCAPLUS

DOCUMENT NUMBER: 142:114074

TITLE: Preparation of polyazido carboxylic acid

esters INVENTOR (S): Dave, Paritosh k.; Duddu, Raja G.; Damavarapu, Reddy;

Gelber, Nathaniel; Yang, Kathy; Surapaneni, C. Rao PATENT ASSIGNEE(S): United States Dept. of the Army, USA U.S., 9 pp.

SOURCE:

CODEN: USXXAM DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 6841690 US 6965042 PRIORITY APPLN. INFO.:	B1 B1	20050111	US 2003-604778 US 2003-604777 US 2002-319801P	P	20030815 20030815 20021219

Y X
$$Z$$
 HO_2C N N N N CO_2H CO_2

This invention relates to a series of novel compds., such as I = N3, AB OH, ONO2, NO2; Y = CH2N3, NO2; A, B = N3, 4-carboxytriazolomethyl], and II [Z = CH2, O, NOH, 2,4-dihydrophenylhydrozono], including

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2-azido-2-azidomethyl-1,3-diazidopropane, 2-azidomethyl-2-hydroxy-1,3diazidopropane, 2-azidomethyl-2-nitrato-1,3-diazidopropane, 2-azidomethyl-2-nitro-1,3-diazidopropane, 2,2-dinitro-1,3-diazidopropane, methallyidiazide, a dimer of methallyidiazide, comprising 3a,8a-bis-azidomethyl-3a,4,8a,9-tetrahydro-3H,8H-bis[1,2,3]triazolo[1,5-a; 1'',5''-d]pyrazine, 1,3-diazidoacetone, and 2-oximido-1,3-diazidopropane. Also shown are reaction intermediates of these compds., including 2,2-bis(chloromethyl)oxirane, and 2,2-bis(azidomethyl)oxirane. In addition, a number of potentially useful energetic compds. have been prepared from the low mol. weight polyazido compds. above, including N-2(azido-1-azidomethyl-ethylidene)-N''-(2,4-dinitrophenyl)-hydrazine (7-DNPH), 1,3-bis(4-carboxytriazolyl)2,2-dinitropropane, tris(4-carboxytriazolomethyl)methanol, benzene-1,3,5-tricarboxylic acid tris(2-azido-1,1-bisazidomethyl-ethyl)ester, adamantane 1,3,5,7-tetracarboxylic acid tetrakis(2-azido-1,1-bisazidomethylethyl)ester, adamantane carboxylic acid (2-azido-1,1-bisazidomethylethyl)ester, cubane 1,3,5,7-tetracarboxylic acid tetrakis (2-azido-1,1-bisazidomethyl-ethyl)ester, cubane 1,4-dicarboxylic acid bis(2-azido-1,1-bisazidomethyl-ethyl)ester. Thus, tris(4carboxytriazolomethyl) methanol (III) was prepared by the reaction of 2-azidomethyl-2-hydroxy-1,3-diazidopropane I [A, B = N3; X = CH2N3; Y = OH] (also prepared) with propiolic acid. 481067-62-3P, 2-Azidomethyl-2-hydroxy-1,3-diazidopropane RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic

RN 481067-62-3 HCAPLUS

CN 2-Propanol, 1,3-diazido-2-(azidomethyl)- (9CI) (CA INDEX NAME)

$$N_3 - CH_2 - CH_2 - N_3$$
 $CH_2 - N_3$
 $CH_2 - N_3$

IT 169564-66-3P, 2-Azidomethyl-2-nitro-1,3-diazidopropane
481067-64-5P, 2-Azido-2-azidomethyl-1,3-diazidopropane
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP
(Preparation)

(preparation of **polyazido** carboxylic acid esters derived from methallyl dichloride)

RN 169564-66-3 HCAPLUS

CN Propane, 1,3-diazido-2-(azidomethyl)-2-nitro- (9CI) (CA INDEX NAME)

RN 481067-64-5 HCAPLUS CN Propane, 1,2,3-triazido-2-(azidomethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c} {\rm N_3} \\ {\rm N_3-CH_2-} \\ {\rm C-CH_2-N_3} \\ {\rm CH_2-N_3} \end{array}$$

THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS REFERENCE COUNT: 6

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:137939 HCAPLUS

DOCUMENT NUMBER: 140:357709

TITLE: Preparation of cage molecule based polyazido

core units for dendrimer synthesis

AUTHOR (S): Dave, Paritosh, Ray, Duddu, Raja; Yang, Kathy;

Damayarapu, Reddy; Gelber, Nathaniel; Surapaneni, Rao;

Gilardi, Richard

CORPORATE SOURCE: GEO-CENTERS, INC. at ARDEC, Picatinny Arsenal, NJ,

07806-5000, USA

Tetrahedron Letters (2004), 45(10), 2159-2162 SOURCE:

CODEN: TELEAY; ISSN 0040 4039

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal LANGUAGE: English

Core mols. based on benzene-, cubane-, and adamantane-polycarboxylates AB with peripheral polyazido substitution were prepared The first synthesis of 1,3-diazidoacetone and its conversion to the corresponding oxime, DNPH, and 2,2-dinitro derivs. is also reported. All azido compds. should be considered dangerous and proper precautions should be taken

during handling and storage of these mols.

ΙT 481067-62-3P

> RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of peripheral polyazido and benzene and cubane and adamantane core unit cages for triazole and tetrazole containing dendrimer synthesis)

RN 481067-62-3 HCAPLUS

2-Propanol, 1,3-diazido-2-(azidomethyl) - (9CI) (CA INDEX NAME) CN

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:605702 HCAPLUS

DOCUMENT NUMBER: 138:75615

TITLE: Novel polyazido/polynitrato compounds

derived from methallyl dichloride

AUTHOR (S): Surapaneni) Rao; Damavarapu, Reddy; Duddu, Raja;

Paritosh R.; Gilardi, Richard D.

CORPORATE SOURCE: US Army Armament Research Development and Engineering

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Center, Picatinny Arsenal, NJ, 07806-5000, USA SOURCE:

International Annual Conference of ICT (2002),

33rd(Energetic Materials), 147/1-147/5

CODEN: IACIEQ; ISSN: 0722-4087

PUBLISHER: Fraunhofer-Institut fuer Chemische Technologie

Journal DOCUMENT TYPE:

LANGUAGE: English

AB Several polynitrato and polyazido compds., derived from a lower homolog of pentaerythritol and have one less methylene unit, were synthesized in order to develop lead-free primary explosives. The compds. were derived from methallyl dichloride by such reactions as epoxidn., nucleophilic substitution, and ring-opening nitration. Nitration. These compds. are of potential interest as energetic plasticizers and their multiple functional groups can be exploited to prepare novel dendritic structures.

IT 481067-62-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(synthesis and reactions of; novel polyazido-polynitrato compds. derived from methallyl dichloride by epoxidn., nucleophilic substitution, and ring-opening nitration)

481067-62-3 HCAPLUS

2-Propanol, 1,3-diazido-2-(azidomethyl)- (9CI) (CA INDEX NAME) CN

$$\begin{array}{c} \text{OH} \\ \text{N}_3 - \text{CH}_2 - \begin{array}{c} \text{C---} \text{CH}_2 - \text{N}_3 \\ \text{CH}_2 - \text{N}_3 \end{array}$$

IT 481067-64-5P

> RL: SPN (Synthetic preparation); PREP (Preparation) (synthesis of; novel polyazido-polynitrato compds. derived from methallyl dichloride by epoxidn., nucleophilic substitution, and ring-opening nitration)

RN 481067-64-5 HCAPLUS

CN Propane, 1,2,3-triazido-2-(azidomethyl)- (9CI) (CA INDEX NAME)

$$n_3 - Ch_2 - Ch_2 - n_3$$
 $Ch_2 - N_3$

=> d l16 ibib abs tot

L16 ANSWER 1 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:101293 HCAPLUS

DOCUMENT NUMBER: 136:118216

TITLE: Alcohol nitrates containing amide, dinitromethylene

> and nitroamine groups, method of preparing them, 3-[(acylamino)dinitroalkyl]oxazolidines and

> 3-[(acylamino)dinitroalkyl]tetrahydrooxazines, and

method of preparing them

INVENTOR(S): Korepin, A. G.; Galkin, P. V.; Perepelkina, E. K.;

Glushakova, N. M.; Eremenko, L. T.; Eremenko, I. L.

PATENT ASSIGNEE(S): Institut Khimicheskoi Fiziki v Chernogolovke RAN,

Russia

SOURCE: Russ., No pp. given

CODEN: RUXXE7

DOCUMENT TYPE:

GI

Patent Russian

LANGUAGE: FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
RU 2146243	C1	20000310	RU 1998-107605	19980422 <
PRIORITY APPLN. INFO.:			RU 1998-107605	19980422

ACNHCH₂C (NO₂) ₂CH₂N

AB R1CONR2(CH2)nC(NO2)2CH2N(NO2)(CH2)mONO2 (I; R1 = Me, 3-nitrophenyl; R2 = H, CH2OH; n = 1, 2; m = 2, 3) were prepared by nitration of 3-[(acylamino)dinitroalkyl]oxazolidines and 3-[(acylamino)dinitroalkyl]tetrahydrooxazines. Prepns. of the oxazolidines and tetrahydrooxazines were also described. Thus, I (R1 = Me, R2 = CH2OH, n = 1, m = 2) was prepared by treatment of oxazolidine II with 90-100% HNO3 at 10° for 2 h; II was prepared by reaction of AcNHCH2CH(NO2)2 with 2-aminoethanol and 30% formalin. The cardioprotectant activity of 3 tested I in mice was comparable to that of N-(2-nitroxyethyl)nicotinamide.

L16 ANSWER 2 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

ΙI

ACCESSION NUMBER:

2001:557548 HCAPLUS

DOCUMENT NUMBER:

135:318467

TITLE:

N-Substituted tetrahydro-1,3-oxazines and oxazolidines

1. A new version of the Mannich reaction involving

amino alcohols

AUTHOR(S):

Korepin, A. G.; Galkin, P. V.; Glushakova, N. M.; Lagodzinskaya, G. V.; Loginova, M. V.; Lodygina, V.

P.; Eremenko, L. T.

CORPORATE SOURCE:

Institute of Problems of Chemical Physics, Russian Academy of Sciences, Chernogolovka, 142432, Russia

SOURCE:

Russian Chemical Bulletin (Translation of Izvestiya

Akademii Nauk, Seriya Khimicheskaya) (2001),

50(1), 104-109

CODEN: RCBUEY; ISSN: 1066-5285 Kluwer Academic/Consultants Bureau

DOCUMENT TYPE:

PUBLISHER:

Journal English

LANGUAGE: OTHER SOURCE(S):

CASREACT 135:318467

GΙ

Mannich reactions of amino alcs. 3-aminopropan-1-ol or 2-aminoethanol with AB HCHO and C-H or N-H acids gave N-substituted tetrahydro-1,3-oxazines or oxazolidines. Thus, reaction of H2NCH2CH2CH2CH (I) with HCHO and 1,1-dinitroethane or 2-bromo-2,2-dinitroethanol gave the 1,3-oxazines II (R = Me, Br). Similar reaction of I with H2NCOCONH2 and H2NCOCH2CH2CONH2 gave the bis(oxazinyl) diamides III (X = bond, CH2CH2), and reaction of H2NCH2CH2OH with HCHO and benzotriazole gave the oxazolylmethylbenzotriazole IV.

REFERENCE COUNT:

THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS 13 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 3 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

1999:661817 HCAPLUS

DOCUMENT NUMBER:

132:35450

TITLE:

Synthesis of β -nitroamino derivatives of

gem-dinitroalkanes

AUTHOR (S):

Tartakovsky, V. A.; Ermakov, A. S.; Varfolomeeva, O.

CORPORATE SOURCE:

N. D. Zelinsky Institute of Organic Chemistry, Russian

Academy of Sciences, Moscow, 117913, Russia

SOURCE:

Russian Chemical Bulletin (Translation of Izvestiya

Akademii Nauk, Seriya Khimicheskaya) (1999),

48(7), 1385-1387

CODEN: RCBUEY; ISSN: 1066-5285

PUBLISHER:

Consultants Bureau

DOCUMENT TYPE:

Journal

LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 132:35450

A method for the synthesis of β -nitroamino derivs. of

gem-dinitroalkanes by nitration of the products of condensation of sulfamic acid derivs. with the corresponding gem-dinitroalkanes is

presented.

REFERENCE COUNT:

5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 4 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

1998:666542 HCAPLUS

DOCUMENT NUMBER:

130:15525

TITLE:

Thermal decomposition of organic azides in propellants

AUTHOR (S): Jin, Shaohua; Li, Wen; Song, Quançai

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Page 31

CORPORATE SOURCE: College of Chemical Engineering and Materials, Beijing

Institute of Technology, Beijing, 100081, Peop. Rep.

China

SOURCE: Hanneng Cailiao (1998), 6(3), 123-127

CODEN: HACAFQ; ISSN: 1006-9941

PUBLISHER: Hanneng Cailiao Bianjibu

DOCUMENT TYPE: Journal LANGUAGE: Chinese

AB The thermal decomposition of 11 compds. containing azidomethyl-gem-dinitro groups

was studied by DTA, and the formal kinetic parameters E and A were obtained. Comparison of the kinetic parameters of some azides with those of trinitromethyl compds. with structures similar to the corresponding compds. shows that E values increase due to the introduction of azide-group. The influences of the number and position of azidomethyl-gem-dinitro groups on the thermal decomposition kinetic parameters of azidomethyl derivs. were also studied.

L16 ANSWER 5 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1998:492697 HCAPLUS

DOCUMENT NUMBER: 129:202675

TITLE: Synthesis and nitration of N,N'-diacyl-2-nitro-1,1-

alkanediamines

AUTHOR(S): Terpigorev, A. N.; Germanova, G. V.; Bazanov, A. G.

CORPORATE SOURCE: Prikladnaya Khimiya Russian Scientific Center, St.

Petersburg, 197198, Russia

SOURCE: Russian Journal of Organic Chemistry (Translation of

Zhurnal Organicheskoi Khimii) (1997),

33(12), 1712-1720

CODEN: RJOCEQ; ISSN: 1070-4280

PUBLISHER: MAIK Nauka/Interperiodica Publishing

DOCUMENT TYPE: Journal LANGUAGE: English

AB Reactions of primary and secondary nitroalkanes with N,N'-bis(ethoxycarbonyl) formamidine and N,N'-diacylformamidines generated in

situ from the corresponding acylamine, tri-Et orthoformate, and 1,1-dinitroethane result in formation of N,N'-diacyl-2-nitro-1,1-

alkanediamines. Methyl-N-nitroamine and 2-fluoro-2,2-dinitroethanol react with N,N'-bis(ethoxycarbonyl)formamidine to give N2-ethoxycarbonyl-N1-

methyl-N1-nitroformamidine and 2-fluoro-2,2-dinitroethyl

N-ethoxycarbonylformimidate, resp. Nitration of N,N'-diacyl-2-nitro-1,1-alkanediamines, depending on the conditions and the number of nitro groups, leads to N,N'-dinitro- or N-mononitro derivs. or is accompanied by

decomposition into polynitroalkanes and Et N-nitrocarbamate.

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 6 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1998:357787 HCAPLUS

DOCUMENT NUMBER: 129:56114

TITLE: Comparison of thermal stabilities of azidomethyl

gem-dinitromethyl compounds and trinitromethyl

compounds

AUTHOR(S): Hong, Yan; Guan, Xiao-Pei; Chen, Bo-Ren

CORPORATE SOURCE: Department of Chemistry and Environmental Engineering,

Beijing Polytechnic University, Beijing, 100022, Peop.

Rep. China

SOURCE: Proceedings of the International Pyrotechnics Seminar

(1995), 21st, 312-315

CODEN: PPYSD7; ISSN: 0270-1898

PUBLISHER: IIT Research Institute

DOCUMENT TYPE: Journal LANGUAGE: English

AB The thermal decomposition characteristics of azidomethyl gem-dinitromethyl

compds. [characterized by the -C(NO2)2CH2N3 group] and trinitromethyl compds. [the C(NO2)3 group] were studied by DTA, and their kinetic

parameters were reported. The azidomethyl gem-dintromethyl compds. have higher thermal stabilities than the corresponding trinitromethyl compds.

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 7 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1998:319646 HCAPLUS

DOCUMENT NUMBER: 129:67758

TITLE: Chloride-assisted nitrolysis of cyclic tertiary amines

AUTHOR(S): Cliff, Matthew D.

CORPORATE SOURCE: Aeronautical and Maritime Research Laboratory

(AMRL)-DSTO, Salisbury, 5108, Australia

SOURCE: Heterocycles (1998), 48(4), 657-669

CODEN: HTCYAM; ISSN: 0385-5414

PUBLISHER: Japan Institute of Heterocyclic Chemistry

DOCUMENT TYPE: Journal LANGUAGE: English

GI

 $\begin{array}{c|c}
NNO_2 \\
HN & NH \\
N & NO_2
\end{array}$

AB Nitramines, e.g. nitrotriazine I (R = NO2), were prepared from tertiary amine heterocycles, e.g. alkyltriazines I (R = Me3C, Me2CH, cyclohexyl, benzyl, Bu, Pr) via a chloride-assisted nitrolysis [HNO3/NH4Cl]. The process is effective for heterocyclic systems containing a single tertiary amine moiety and gives good to excellent yields for primary, secondary and tertiary alkyl leaving groups. Heterocyclic systems containing two tertiary amines, e.g. hexahydropyrimidines II (R1 = Me3C, Me2CH, cyclohexyl), are best nitrated via a tert-Bu leaving group, with other alkyl moieties leading to ring-opened species O2NNR1CH2C(NO2)2CH2NR1NO upon treatment with nitrating media both in the presence and absence of chloride ions.

REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 8 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1997:738022 HCAPLUS

DOCUMENT NUMBER: 128:75024

TITLE: Thermal studies of 2-azido-1,1-dinitroethyl compounds

and trinitromethyl compounds

AUTHOR(S): Yan, Hong; Guan, Xiao-Pei

CORPORATE SOURCE: Department of Chemistry and Environmental Engineering,

Beijing Polytechnic University, Beijing, 100022, Peop.

Rep. China

PUBLISHER:

SOURCE: Journal of Energetic Materials (1997),

15(4), 283-288

CODEN: JOEMDK; ISSN: 0737-0652 Dowden, Brodman & Devine, Inc.

DOCUMENT TYPE: Journal LANGUAGE: English

AΒ The thermal decomposition characteristics of 2-azido-1,1-dinitrocthyl [-C(NO2)2CH2N3] compds. and trinitromethyl [-C(NO2)3] compds. have been studied by DTA, and their kinetic parameters are also reported. results indicate that these 2-azido-1,1-dinitroethyl compds. have higher thermal stability relative to the corresponding trinitromethyl compds.

REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 9 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1997:415029 HCAPLUS

DOCUMENT NUMBER: 127:95011

TITLE: Synthesis of 3-azido-2,2-dinitropropyl-substituted

nitramines

AUTHOR(S): Yan, Hong; Guan, Xiao-Pei

CORPORATE SOURCE: Dep. Chem. and Environmental Engineering, Beijing

Polytechnic Univ., Beijing, 100022, Peop. Rep. China

SOURCE: Youji Huaxue (1997), 17(3), 284-288

CODEN: YCHHDX; ISSN: 0253-2786

PUBLISHER: Kexue DOCUMENT TYPE: Journal LANGUAGE: Chinese

Title azides MeN(NO2)CH2C(NO2)2CH2N3, [CH2N(NO2)CH2C(NO2)2CH2N3]2, and O2NN[CH2C(NO2)2CH2N3]2 were prepared from alcs. MeN(NO2)CH2C(NO2)2CH2OH,

[CH2N(NO2)CH2C(NO2)2CH2OH]2, and O2NN[CH2C(NO2)2CH2OH]2 via the

corresponding triflats.

L16 ANSWER 10 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1996:666292 HCAPLUS

DOCUMENT NUMBER: 125:304561

TITLE: Synthesis and characteristics of high energy density

azidonitramine additives

AUTHOR (S): Qu, Yuxiang; Chen, Boren; Yan, Hong; Dong, Shu'an CORPORATE SOURCE: Sch. Chemical Eng. Maters. Sci., Beijing Inst.

Technol., Beijing, 100081, Peop. Rep. China

SOURCE: Beijing Ligong Daxue Xuebao (1996), 16(2),

121-128

CODEN: BLXUEV; ISSN: 1001-0645

PUBLISHER: Beijing Ligong Daxue Xuebao Bianjibu

DOCUMENT TYPE: Journal LANGUAGE: Chinese

Three novel high-energy-d. gem-dinitro azidonitramines were synthesized by introduction of an azidomethyl group into a nitroform nitramine mol. to replace a nitro group. The synthesized gem-dinitro azidonitramines were identified and characterized. The azidonitramines showed very high d. (1.7-1.8 g/cm3), high nitrogen contents (.apprx.40%), satisfactory oxygen balance (-23% to -35%), high pos. enthalpy of formation (.apprx.500

kJ/mol), and acceptable thermal stability (thermal decomposition temperature

.apprx.200°). These compds. may find applications in

high-energy-d. materials as additives.

L16 ANSWER 11 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1996:514610 HCAPLUS

DOCUMENT NUMBER: 125:172480

TITLE: Synthesis of high density azidonitramines AUTHOR (S): Yan, Hong; Guan, Xiao-Pei; Chen, Bo-Ren

CORPORATE SOURCE: Dep. of Chemistry and Environmental Engineering,

Beijing Polytechnic Univ., Beijing, 100022, Peop. Rep.

China

SOURCE: International Annual Conference of ICT (1996

), 27th (Energetic Materials), 135.1-135.5

CODEN: IACIEQ

PUBLISHER: Fraunhofer-Institut fuer Chemische Technologie

DOCUMENT TYPE: Journal LANGUAGE: English

Three nitramines containing the 2-azido-1,1-dinitroethyl group have been synthesized, one of which, 1,7-diazido-2,2,4,6,6-pentanitro-4-azaheptane, possesses a d. of 1.835 g/cm3. For these compds. the mol. structures have been determined, and some of the properties (e.g., decomposition point) are

also

reported.

L16 ANSWER 12 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

1995:830797 HCAPLUS

DOCUMENT NUMBER:

123:291159

TITLE:

Development of energetic additives for propellants in

China

AUTHOR (S):

Ou, Yuxiang; Chen, Boren; Yan, Hong; Jia, Huiping; Li,

Jianjun; Dong, Shuan

CORPORATE SOURCE:

Department Chemical Engineering, Beijing Institute

Technology, Beijing, 100081, Peop. Rep. China

SOURCE:

Journal of Propulsion and Power (1995),

11(4), 838-47

CODEN: JPPOEL; ISSN: 0748-4658

PUBLISHER: American Institute of Aeronautics and Astronautics DOCUMENT TYPE:

Journal

LANGUAGE: English

The development of energetic azide binders and plasticizers for solid propellants in China was described, focusing on 14 azides. The reaction routes and conditions for preparing these azides were summarized; the performance of the azides, including d., m.p., enthalpy of formation, thermal decomposition temperature (determined by differential scanning calorimetry or

DTA), impact sensitivity, etc, were presented. The azides were arranged in six categories: (1) azide polyethers (glycidyl azide polymer, 3,3-bis(azidomethyl)oxetane (BAMO) homopolymer, and BAMO-tetrahydrofuran copolymer), (2) azidonitramines (1,5-diazido-3-nitrazapentane, N-nitro-N-azidomethyl-gem-dinitroethylmethylamine, and N,N'-bis(azidomethyl-gem-dinitroethyl)ethylenedinitramine), (3) azidonitro compds. [2-nitro-2-methyl-1,3-diazidopropane, 2-nitro-2-azidomethyl-1,3diazidopropane, and 1-azido-2-(2,4,6-trinitrophenyl)ethane], (4) aliphatic azides (1,2,4,triazidobutane and tetraazidomethylemethane), (5) azidonitrates (pentaerythritol diazidodinitrate), and (6) oxygen heterocyclic azides (3-azidomethyl-3-ethyloxetane and 2,2-dimethyl-5azidomethyl-5-nitro-1,3-dioxane).

L16 ANSWER 13 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

1995:698094 HCAPLUS

DOCUMENT NUMBER:

123:339226

TITLE:

Destructive nitration of polynitro carbonyl compounds.

III. Synthesis of 2,2,3,3,3-

pentanitropropylnitrobenzenes and -N-nitroaniline

AUTHOR (S):

Stepanova, O. P.; Golod, E. L.

CORPORATE SOURCE: St. Peterburg. Gos. Tekhnol. Inst., Russia

SOURCE: Zhurnal Organicheskoi Khimii (1994), 30(10),

1521-3

CODEN: ZORKAE; ISSN: 0514-7492

PUBLISHER: Nauka DOCUMENT TYPE: Journal LANGUAGE: Russian

CASREACT 123:339226 OTHER SOURCE(S):

RCH(NO2)2 [R = Ph, 3-O2NC6H4, 2,4-(O2N)2C6H3] added to CH2:CHCOMe (I) in aqueous MeOH to give 70-80% RC(NO2)2CH2CH2COMe (same R), but attempts to convert these to title compds. were unsuccessful. Adding RCH2CH(NO2)2 [R

= Ph, 4-02NC6H4, 2,4-(O2N)2C6H3] to I as above gave 40-86%

RCH2C(NO2)2CH2CH2COMe (same R), which reacted with HNO3-H2SO4 to give

11-19% RCH2C(NO2)2C(NO2)3 (same R). Condensation reaction of

4-O2NC6H4NHCH2OMe with HC(NO2)2CH2CH2COMe in aqueous MeOH to give 37% 4-O2NC6H4NHCH2C(NO2)2CH2CH2COMe, which reacted with HNO3-H2SO4 to give 7%

2, 4-(O2N) 2C6H3N (NO2) CH2C (NO2) 2C (NO2) 3.

L16 ANSWER 14 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1994:326920 HCAPLUS

DOCUMENT NUMBER: 120:326920

TITLE: Calculations of heats of formation for nitramines and

alkyl nitrates with PM3 and MM2

AUTHOR (S): Akutsu, Yoshiaki; Che, Renhao; Tamura, Masamitsu

Fac. Eng., Univ. Tokyo, Tokyo, 113, Japan CORPORATE SOURCE: Journal of Energetic Materials (1993), SOURCE:

11(3), 195-203

CODEN: JOEMDK; ISSN: 0737-0652

DOCUMENT TYPE: Journal LANGUAGE: English

The heats of formation (ΔHf°) for several nitramines and

alkyl nitrates were calculated with the semi-empirical MO theory, PM3, and

with mol. mechanics, MM2. Both methods ests. ΔHf°

accurately. By combining heats of vaporization and sublimation obtained

by the additivity rule with AHf° in the gas phase obtained by PM3 and MM2, ΔHf° in the condensed phase can be estimated

accurately enough for prediction of energy hazards.

L16 ANSWER 15 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

1994:302695 HCAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 120:302695

TITLE: Comparative characteristics of some experimental and

computational methods of estimating impact sensitivity

parameters of explosives

AUTHOR (S): Afanas'ev, German T.; Pivina, Tatyana S.; Sukhachev,

Dimitril V.

CORPORATE SOURCE: Chem. Phys. Inst., Moscow, 117913, Russia '

Propellants, Explosives, Pyrotechnics (1993 SOURCE:

), 18(6), 309-16

CODEN: PEPYD5; ISSN: 0721-3115

DOCUMENT TYPE: Journal LANGUAGE: English

Some theor. and exptl. ests. were presented for the quant. estimate of sensitivity of explosives to mech. impact, using a Logical-Structural

Approach [T. Pivina (1991)] and the Quant. Structure-Property

Relationship, QSPR, [T. Pivina (1992)]. These methods were successful for evaluating and predicting h50% (the impact sensitivity) and Δcr (the detonatable layer). For calcn. of the h50% parameter, the QSPR approach

L16 ANSWER 16 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

1991:493082 HCAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 115:93082

TITLE: Nitro- and fluoropolyformals. III. Copolyformals

from mixtures of fluoro- and nitro- α , ω -

diols

Nock, Lori A.; Goldwasser, Judah M.; Adolph, Horst G. AUTHOR(S):

Energ. Mater. Div., Nav. Surf. Warf. Cent., Silver CORPORATE SOURCE:

Spring, MD, 20903-5000, USA

SOURCE: Journal of Polymer Science, Part A: Polymer Chemistry

(1991), 29(8), 1133-49

CODEN: JPACEC; ISSN: 0887-624X

DOCUMENT TYPE:

Journal

LANGUAGE: English

Polyformals of fluoro-, nitramine-, and C-nitrodiols showed widely differing properties with respect to glass transition temperature (Tq), melting transition, and solubility Polymers with desirable combinations of these properties, e.g., low Tg, high nitro content, and good solubility in polar solvents, were expected to result from acid-promoted copolycondensation of appropriate mixts. of diols with HCHO. A series of such condensations were carried out and the polymers obtained from binary mixts. of fluoroand nitrodiols, different nitrodiols, and fluoro- or nitrodiols and carboranediols, were characterized by gel-permeation chromatog., 1H-NMR, and DSC anal.

L16 ANSWER 17 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

1991:46054 HCAPLUS

DOCUMENT NUMBER:

114:46054

TITLE:

Block copolymers of formaldehyde and

1,2-bis(2-hydroxyethyl)-1,2-dicarbadodecaborane and

polynitroalkyl diols

INVENTOR (S):

Adolph, Horst G.; Nock, Lori A. United States Dept. of the Navy, USA

PATENT ASSIGNEE(S): SOURCE:

Statutory Invent. Regist., 4 pp.

CODEN: SRXXEV

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
_	is prepared from HC	HO and	ck copolymer a diol. mixt	US 1989-389239 US 1989-389239 Useful as a binder for useful as a binder for ure comprising ≤50 mol%	propellants
	(or their mixts.). HOCH2CH2N(NO2)CH2C(such compds., and c 2.74 g HOCH2CH2N(NC 0.140 g 1,2-bis(2-h	The ni NO2)2CH comprise (2)CH2C(lydroxye	trodiols com 2CH2OH, HOCH s the remain NO2)2CH2OCH2 thyl)-1,2-di	decaborane (12) (I) with oprise (HOCH2CH2)2NNO2, M2CH2N(NO2)CH2CH2N(NO2)C oder of the diol mixture M3CH2C(NO2)2CH2N(NO2)CH2 M3Carbadodecaborane (12) M4Carbadodecaborane (12)	CH2CH2OH, and than I. Thus, CH2OH and dissolved in
was		٥,			

added followed by dropwise addition of BF3. Et20. Stirring 15 h at 20°, adding 15 mL CH2Cl2, stirring with 20 mL H2O and 0.5 mL 30%

H2O2 for 3 h, separating the organic phase, stirring with 20 mL 1% aqueous KOH containing

0.25 mL 30% H2O2, separating the organic phase, evaporating CH2Cl2, and triturating

with 25-mL portions of H2O at 35-40° until no sulfolane was detected by NMR gave polymer, which was redissolved in CH2Cl2, and the solution stirred with silica gel overnight, filtered, and evaporated to give 2.2

g (80%) glassy polymer with number-average mol. weight 2160.

L16 ANSWER 18 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

1991:46053 HCAPLUS

DOCUMENT NUMBER:

114:46053

TITLE:

Block copolymers of 1,2-bis(2-hydroxyethyl)-1,2-

dicarbadodecaborane(12) and polyfluoroalkyl diols and

formaldehyde

INVENTOR (S):

Adolph, Horst G.; Nock, Lori A. United States Dept. of the Navy, USA

PATENT ASSIGNEE(S): SOURCE:

Statutory Invent. Regist., 4 pp.

CODEN: SRXXEV

DOCUMENT TYPE:

Patent English

LANGUAGE:

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 784	H1	19900605	US 1989-389217	19890802 <
PRIORITY APPLN. INFO.:			US 1989-389217	19890802
AB A dihydroxy-termin	ated cop	polyformal	formed from HCHO and a	diol comonomer
mixture of <50 mol	% 1,2-bi	is(2-hydrox	yethyl)-1,2-dicarbadode	ecaborane and
balance mixture of	fluoro	diol/nitrod	iol mixture wherein the	e nitrodiol
comprises <50 mol%	(based	on fluorod	iol/nitrodiol mixture).	The fluoroalkyl
diol prepolymers w	ith cark	orane grou	ps are a polymeric bind	ler for
propellants, the c	arborane	e groups wi	ll not migrate or cryst	callize out, and
the burning rates	of prope	ellant comp	osites are controllable	by varying the
carborane content.	- -	_		

L16 ANSWER 19 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

1990:516127 HCAPLUS

DOCUMENT NUMBER:

113:116127

TITLE:

Hydroxy-terminated polyformals of fluorodiols with

nitrodiols

INVENTOR(S):

Nock, Lori A.; Adolph, Horst G.

PATENT ASSIGNEE(S):

United States Dept. of the Navy, USA Statutory Invent. Regist., 5 pp.

SOURCE:

DOCUMENT TYPE:

CODEN: SRXXEV Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 730	H1	19900206	US 1989-389211	19890802 <
PRIORITY APPLN. INFO.:			US 1989-389211	19890802

AB The title polymers, with low glass temps. and useful as binders for explosives and propellants, are prepared from HCHO, fluorinated diols, and nitrodiols. Thus, BF3-catalyzed polymerization of HOCH2(CF2)4CH2OH.6.01, ${\tt HOCH2CH2N\,(NO2)\,CH2CH2N\,(NO2)\,CH2CH2OH}$ 5.46, and s-trioxane 1.38 g in

sulfolane at room temperature overnight gave a polyacetal with number-average mol. weight

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2080, weight-average mol. weight 3300, and OH equivalent weight 113 by 19F-NMR.

L16 ANSWER 20 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1988:97345 HCAPLUS

DOCUMENT NUMBER: 108:97345

TITLE: 1,9-difluoro-1,1,3,5,7,9,9-octanitro-3,7-diazanonane

and method of preparation as energetic oxidizer

INVENTOR(S): Frankel, Milton B.; Witucki, Edward F.

PATENT ASSIGNEE(S): Rockwell International Corp., USA

SOURCE: U.S., 3 pp.

CODEN: USXXAM DOCUMENT TYPE: Patent

LANGUAGE: Patent English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

US 4701557 A 19871020 US 1982-407198 19820811 <-PRIORITY APPLN. INFO.: US 1982-407198 19820811

OTHER SOURCE(S): CASREACT 108:97345

AB 1,9-Difluoro-1,1,3,5,5,7,9,9-octanitro-3,7-diazanonane (I) is synthesized as a energetic oxidizer for propellants by reacting 2-fluoro-2,2-dinitroethylamine with 2,2-dinitro-1,3-propandiol and treating the resulting white solid with HNO3 and H2SO4. I was obtained in 48% yield and had m.p. 139-140° after recrystn. from ClCH2CH2Cl. I has impact sensitivity 44 in.-lb, endotherm onset 136° and peak 138°, and exotherm onset 160° and peak 204°, and is a viable replacement for HMX or NH4ClO4.

L16 ANSWER 21 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1987:478355 HCAPLUS

DOCUMENT NUMBER: 107:78355

TITLE: Synthesis of polyformals from nitro- and fluorodiols.

Substituent and chain-length effects

AUTHOR(S): Adolph, Horst G.; Goldwasser, Judah M.; Koppes,

William M.

CORPORATE SOURCE: Energetic Mater. Div., Naval Surf. Weap. Cent., Silver

Spring, MD, 20903-5000, USA

SOURCE: Journal of Polymer Science, Part A: Polymer Chemistry

(1987), 25(3), 805-22

CODEN: JPACEC; ISSN: 0887-624X

DOCUMENT TYPE: Journal LANGUAGE: English

AB A series of primary and secondary diols carrying nitroalkyl, NO2, and F substituents was reacted with HCHO under conditions of acid catalysis. Short-chain primary diols gave cyclic formals while predominantly linear polymers were obtained beginning with 1,5-pentanediols and 1,6-hexanediols, depending upon the nature of the substituents. No polymers were formed from secondary diols with 1-nitroalkyl substituents. The effect of monomer structure on polymer formation was discussed. The polymers were characterized by gel permeation chromatog. and end-group anal.

L16 ANSWER 22 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1986:88995 HCAPLUS

DOCUMENT NUMBER: 104:88995

TITLE: Synthesis of novel polynitrodiols

AUTHOR(S): Koppes, William M.; Sitzmann, Michael E.; Adolph,

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CORPORATE SOURCE: Energetic Mater. Div., Nav. Surface Weapons Cent.,

Silver Spring, MD, 20903-5000, USA

SOURCE: Journal of Chemical and Engineering Data (1986

), 31(1), 119-23

CODEN: JCEAAX; ISSN: 0021-9568

DOCUMENT TYPE: Journal LANGUAGE:

English

OTHER SOURCE(S): CASREACT 104:88995

The synthesis of a number of polynitroalkanediols of widely varying structure is reported. Several of the synthesis methods described constitute novel variations or improvements of known reactions: some polynitroaliph. carboxylic acids undergo the Schmidt reaction only in triflic acid as reaction medium; 3-nitropropyl acetate [21461-49-4] was advantageously prepared by a variation of the Kornblum reaction with aqueous Me2SO as solvent; 3,3-dinitropropanol was obtained by an intramol. variant of the alkaline

L16 ANSWER 23 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1983:522404 HCAPLUS

DOCUMENT NUMBER: 99:122404

nitration method.

TITLE: Synthesis of 1,3,5,5-tetranitrohexahydropyrimidine

AUTHOR (S): Levins, D. A.; Bedford, C. D.; Staats, S. J. CORPORATE SOURCE: SRI Int., Menlo Park, CA, 94025, USA

SOURCE: Propellants, Explosives, Pyrotechnics (1983)

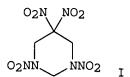
), 8(3), 74-6

CODEN: PEPYD5; ISSN: 0721-3115

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 99:122404

GI



AB The title compound I was prepared in 37% yield by nitration of 1,3-diisopropyl-5,5-dinitrohexahydropyrimidine, prepared in 88% yield by cycloaddn. of Me2CHNH2 to HOCH2C(NO2)2CH2OH, with 95% HNO3 1.5 h at 0° and allowing the mixture to stand overnight at room temperature Addnl. obtained were 24% Me2CHN(NO)CH2C(NO2)2CH2N(NO)CHMe2 and Me2CHN (NO2) CH2CH (NO2) 2.

L16 ANSWER 24 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1979:559853 HCAPLUS

DOCUMENT NUMBER: 91:159853

TITLE: The relationship of impact sensitivity with structure

of organic high explosives. I. Polynitroaliphatic

explosives

AUTHOR (S): Kamlet, Mortimer J.

CORPORATE SOURCE: White Oak Lab., Nav. Surf. Weapons Cent., Silver

Spring, MD, 20910, USA

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SOURCE: Off. Nav. Res., [Tech. Rep.] ACR (U. S.) (1976

), ACR-221, Proc. Symp. (Int.) Detonation, 6th, 312-22

CODEN: OFNRAZ; ISSN: 0500-2001

DOCUMENT TYPE: Report LANGUAGE: English

AB Impact sensitivities of organic high explosives are primarily functions of their thermal decomposition rates at the temps. generated under the impact hammer. For classes of explosives with similar decomposition mechanisms, there appear to be rough linear relationships (sensitivity-structure trends) between logarithmic 50% impact heights and values of OB100, a measure of oxidant balance. Polynitroaliph. explosives containing at least one N-nitro linkage are more sensitive as a class than nitroaliph. explosives containing only C-nitro linkages.

L16 ANSWER 25 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1979:103135 HCAPLUS

DOCUMENT NUMBER: 90:103135

TITLE: Evaluation of enthalpies of atomization in CNDO/2

calculations

AUTHOR (S): Belik, A V.; Shlyapochnikov, V. A.

CORPORATE SOURCE: Inst. Org. Khim. im. Zelinskogo, Moscow, USSR

SOURCE: Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (

1977), (12), 2795-8 CODEN: IASKA6; ISSN: 0002-3353

DOCUMENT TYPE: Journal LANGUAGE: Russian

Coeffs. (K) relating resonance energies of bonds to the enthalpies of ΑB atomization (ΔH) were determined for several bond types by comparing the calculated and exptl. ΔH for numerous small mols. The K values were then used to calculate ΔH for several nitro compds. The calculated values agreed satisfactorily with exptl. data.

L16 ANSWER 26 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1977:170597 HCAPLUS

DOCUMENT NUMBER: 86:170597

TITLE: Steric effects in molecules of mono- and

polynitroalkanes

AUTHOR (S): Pivina, T. S.; Gritsaev, E. I.; Smirnov, B. B.;

Shlyapochnikov, V. A.; Novikov, S. S.

CORPORATE SOURCE: Inst. Org. Khim. im. Zelinskogo, Moscow, USSR

SOURCE: Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (

1977), (1), 182-4 CODEN: IASKA6; ISSN: 0002-3353

DOCUMENT TYPE: Journal LANGUAGE: Russian

Equilibrium NO2-group angles, strain energies, and heats of atomization were calculated for C1-C4 alkanes containing 1-8 NO2 groups. A steric parameter was calculated which could predict the stability of the mol. The steric effects arising from the NO2 groups increased nonlinearly with the number of NO2 groups and with the length of the C chain.

L16 ANSWER 27 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1973:505216 HCAPLUS

DOCUMENT NUMBER: 79:105216

TITLE: Cyclic derivatives of 3-fluoro-3,3-dinitro-1-

aminopropane

Sviridov, S. I.; Gafurov, R. G.; Korepin, A. G.; AUTHOR (S):

Eremenko, L. T.

CORPORATE SOURCE: Inst. Khim. Fiz., Moscow, USSR

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Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (SOURCE:

1973), (6), 1369-71

CODEN: IASKA6; ISSN: 0002-3353

DOCUMENT TYPE: Journal LANGUAGE: Russian

GI For diagram(s), see printed CA Issue.

FC(NO2)2CH2CH2NH2 (RNH2 in following) and formalin gave I which with AB

Ac20-HNO3 gave RN(NO2)CH2OAc. RNH2 and 9% formalin with KHC(NO2)2 in aqueous EtOH at pH 4-5 gave II, which with HNO3 gave RN(NO2)CH2 2C(NO2)2, also formed from III (prepared from RNH2 and formalin with KHC(NO2)2 in aqueous medium at pH 5.5). II and III did not yield any unsym. ring opening

products in reactions with HNO3.

L16 ANSWER 28 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

CORPORATE SOURCE:

1973:504674 HCAPLUS

DOCUMENT NUMBER:

79:104674

TITLE:

New derivatives of 3,3,3-trinitro-1-aminopropane and

their nitrolysis

AUTHOR (S):

Gafurov, R. G.; Sviridov, S. I.; Eremenko, L. T.

Inst. Khim. Fiz., Moscow, USSR

SOURCE:

Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (

1973), (6), 1366-9

CODEN: IASKA6; ISSN: 0002-3353

DOCUMENT TYPE:

Journal Russian

LANGUAGE:

For diagram(s), see printed CA Issue. GI

AB KCH(NO2)2 and 30% formalin in aqueous EtOH at pH 6 were slowly treated with RNH2.HCl R = (O2N)3CCH2CH2 to form I. In aqueous system at pH 5.5 the

product was II while at pH 7.5-8 it was RNHCH2C(NO2)2CH2N+HRCH2C(NO2)2-

(III). I and HNO3 gave RN(NO2)CH2CH(NO2)2 which brominated to

RN(NO2)CH2CBr(NO2)2, also formed from II and III by treatment with Br2,

followed by HNO3-H2SO4. III and mixed acid gave

RN(NO2)CH2C(NO2)2CH2NRCH2CH(NO2)2, which brominated to

RN(NO2)CH2C(NO2)2CH2NRCH2CBr(NO2)2, while mixed acid at 90° gave

RN(NO2)CH2 2C(NO2)2. This also formed from I or II with mixed acid at

elevated temperature

L16 ANSWER 29 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

1973:404971 HCAPLUS

DOCUMENT NUMBER:

79:4971

TITLE:

Amidomethylation of alkali salts of polynitroalkanes

AUTHOR (S):

Ivanov, P. A.; Popov, E. I.; Selivanov, V. F.;

Gidaspov, B. V.

CORPORATE SOURCE:

Leningr. Tekhnol. Inst. im. Lensoveta, Leningrad, USSR

SOURCE: Zhurnal Organicheskoi Khimii (1972), 8(11),

2371-3

CODEN: ZORKAE; ISSN: 0514-7492

DOCUMENT TYPE:

Journal

LANGUAGE:

Russian

Alkylation of K or Na salts of RCH(NO2)2 [R = H, cyano, Me(O2N)NCH2,

m-O2NC6H4, MeOCH2, NO2, Br] with BzNHCH2Cl in anhydrous Me2CO gave 80-96%

BzNHCH2C(NO2)2R.

L16 ANSWER 30 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

1973:123728 HCAPLUS

DOCUMENT NUMBER:

78:123728

TITLE:

Principles of the thermal decomposition of

 β -polynitroalkyamines and amides

AUTHOR (S):

Selivanov, V. F.; Vlasenko, I. V.; Stepanov, R. S.;

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Gidaspov, B. V. CORPORATE SOURCE: Leningrad, USSR

Gorenie Vzryv, Mater. Vses. Simp., 3rd (1972 SOURCE:

), Meeting Date 1971, 789-93. Editor(s): Stesik, L. N. "Nauka": Moscow,

USSR.

CODEN: 26JOAP DOCUMENT TYPE: Conference LANGUAGE: Russian

Rate consts. and activation parameters were determined for the thermal decomposition

of (1) RC6H4NHCH2CMe(NO2)2 (R = H, 0- and p-Me, 0- and p-Cl, m- and p-NO2) (2) RC6H4NHCH2C(NO2)2 - CH2CMe(NO2)2 (R = H, p-Me, p-Cl, m- and p-NO2), (3) AcN- HCHRC(NO2)3 [R = H, alkyl, Ph, PhCH2, CH2CH2C(NO2)3, CH2C1], and (4) BzNHCH2C(NO2)2C(N2)2R (R = CN, NO2, ClH, CH2CH2CO2Me, Me, Et) in di-Bu phthalate or trinitrotoluene. The 4 types of compds. decomposed by the same mechanism, the 1st and rate-determining step of which was heterolyutic cleavage of the CH-NH bond to form a carbonium-immonium cation and an anion of a polynitro compound

L16 ANSWER 31 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1967:453645 HCAPLUS

DOCUMENT NUMBER: 67:53645

Preparation of nitro aza diisocyanates suitable as TITLE:

explosives

INVENTOR(S): Vanneman, Clinton R.; Klager, Karl

PATENT ASSIGNEE(S): Aerojet-General Corp.

Ger., 3 pp.
CODEN: GWXXAW SOURCE:

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. APPLICATION NO. KIND DATE DATE -------------------19670420 DE

AΒ An outline of the synthesis of the title compds. (I) is given. Nitro aza dicarboxylic acids (II) were prepared either by hydrolysis of the corresponding nitro aza dinitriles or by condensation of a nitro diol with an amino ester, followed by HNO3 oxidation The various II were converted to the corresponding acid chlorides (III) with SOCl2. Treatment of III with NaN3, KN3, or Mg(N3)2 at 0-5° gave the corresponding azides, which were converted to I by a Curtius rearrangement. Thus, a solution of 11 g. 4,7,7,10-tetranitro-4,10-diaza-1,13-tridecanedicarbonyl chloride in 50 ml. Me2CO was added dropwise to a solution of 4.6 g. NaN3 in 15 ml. H2O (kept at 5°). The mixture was stirred 1 hr. at 0° and filtered. The residue was washed with H2O and (CH2Cl2)2 and dried in vacuo to give 3,6,6,9-tetranitro-3,9-diazaundecamethylene diisocyanate, m. 88-90°

L16 ANSWER 32 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1963:461451 HCAPLUS

DOCUMENT NUMBER: 59:61451 ORIGINAL REFERENCE NO.: 59:11236b-g

TITLE: Synthesis and reactions of trinitromethyl compounds

AUTHOR (S): Frankel, M. B.

Stanford Res. Inst., Menlo Park, CA CORPORATE SOURCE: SOURCE: Tetrahedron (1963), 19(Suppl. 1), 213-17

CODEN: TETRAB; ISSN: 0040-4020

DOCUMENT TYPE: Journal LANGUAGE: Unavailable

As systematic study of the synthesis of trinitromethyl compds. from HC(NO2)3 and (O2N)3CCH2OH (I) is summarized. HC(NO2)3 adds readily in a Michael type of addition to α,β -unsatd. compds. such as H2C:CHCO2H and its esters, HOCH2COCH:CH2, and O2NCH:CH2 to yield 83% (NO2)3CCH2CH2CO2CH, m. 61°; 64% (NO2)3CCH2CH2CO2CH:CH2, b6 85-9°, n25D 1.4707; 71% (NO2)3CCH2CH2CO2CH2- CH:CH2, b0.3 71-2°, n25D 1.4676; 74% (NO2)3CCH2CH2CO- CH2OH, m. 77°; and 50% (NO2)3CCH2CH2NO2, m. 50-1°. Of special interest was addition of HC(NO2)3 to H2C:C(NO2)CH2OAc (II). Condensation of MeNO2 with HCHO in the presence of NaOH gave the acid Na salt, HOCH2C(: NO2Na)CH2OH, which was acidified and acetylated to give AcOCH2CH(NO2)CH2OAc, and converted by vapor phase cleavage at $180^{\circ}/100$ mm. to II. Addition of MeCH(NO2)2 to II gave MeC(NO2)2CH2CH(NO2)CH2C(NO2)2Me, and in similar manner, addition of HC(NO2)3 to II yielded (NO2)3CCH2CH(NO2)CH2C(NO2)3. It was of interest to determine the various types of trinitromethyl compds. that could be prepared

from

(NO2)3CCH2CH2CO2H (III). III refluxed 4 hrs. with SOC12 yielded 33% [(NO2)3CCH2CH2CO]2O, m. 109-10°, but 20 hrs. refluxing gave 82% (NO2)3CCH2CH2COCl (IV), b0.5 65-6°, n25D 1.4835. IV treated with NaN3 gave the azide, converted in situ to 71.2% (NO2)3CCH2CH2NCO (V), b10 73-5°, n25D 1.4805. V hydrolyzed with HCl yielded 94% (NO2)3CCH2CH2NH2.HCl (VI), m. 161-3°. V and VI were used for the preparation of trinitromethyl carbamates (VII) and trinitromethylamines (VIII). VII were prepared by addition of I to various isocyanates and the addition of different alcs. to V. I is considerably more acidic than ordinary alcs. and reacts less readily with isocyanates. I refluxed with an isocyanate in CHCl3 several hrs. in the presence of a catalytic amount of ferric acetonylacetonate gave essentially quant. yields of the tabulated VII. All were nitrated to the corresponding N-nitro derivs. VIII were prepared by the Mannich condensation of I with various primary amines and the reaction of VI with nitro alcs. Since nitro alcs. are demethylolated in the presence of base, the condensations were carried out by portionwise addition of an equivalent amount of base to VI and nitro alc. in H2O with immediate precipitation

of the tabulated VIII. All these secondary amines were nitrated to the corresponding nitramines. The reaction of (HOCH2)2C(NO2)2 with VI and HCHO yielded 40.8% 1,3-bis-(3,3,3-trinitropropyl)-5,5dinitroperhydropyrimidine, m. 119-21°. Condensation of VI with HCHO gave a quant. yield of 1,3,5-tris(3,3,3-trinitropropyl)perhydro-1,3,5triazine, m. 121-3°. Esters of I were prepared according to the procedure of Hill (CA 49, 8103f) by treating the acid chlorides with I in the presence of a catalytic amount of AlCl3. The esterification of 4,4,6,6,8,8-hexanitroundecanedioic acid was carried out in 100% H2SO4 as the ionizing solvent. The 2,2,2-trinitroethyl esters prepared are summarized (ester, % yield, and m.p. given): N(NO2)[CH2CO2CH2C(NO2)3]2, 77.8, 160.0-60.5°; N(NO2)[CH2CH2CO2CH2C(NO2)3]2, 35.9, 110-11°; [CH2N(NO2)CH2CO2CH2C(NO2)3]2, 5.6, 195-7°; [CH2N(NO2)CH2CH2CO2CH2C(NO2)3]2 85.5, 126-8°; MeC(NO2)2CH2N(NO2)CH2CO2CH2C(NO2)3, 50.3, 121.0-1.5°; C(NO2) 2 [CH2CH2CO2CH2C(NO2) 3] 2, 47.0, 170-1°; C-(NO2)2[CH2C(NO2)2CH2CH2CO2CH2C(NO2)3]2, 87.8, 117-18°.

L16 ANSWER 33 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1963:461424 HCAPLUS

DOCUMENT NUMBER: 59:61424
ORIGINAL REFERENCE NO.: 59:11228c-f

TITLE: Preparation of polynitro compounds by the Michael

condensation and the Mannich reaction

AUTHOR(S): Hamel, E. E.

CORPORATE SOURCE: Aerojet-Gen., Sacramento, CA

SOURCE: Tetrahedron (1963), 19(Suppl. 1), 85-95

CODEN: TETRAB; ISSN: 0040-4020

DOCUMENT TYPE: Journal LANGUAGE: Unavailable

The Michael condensation for the preparation of polynitro compds., where the AR addenda contained one or more terminal NO2 groups, proceeded smoothly at 20-50° in aqueous MeOH and required no catalyst when the nitro compound was used as its Na or K aci salt. The expected product was obtained in all but two of the systems studied. Reaction of 2 moles H2C:CHCO2Me with O2NC(: NO2K)CH2C(: NO2K)NO2 gave only the monoadduct O2NC(: NO2K) CH2C(O2N) 2CH2CH2CO2Me. RN[CH2C(NO2): NO2K] 2-(I, R = H) (II) (1 mole) and 2 moles H2C: CHCO2Me at 20-30° in aqueous MeOH gave 81% (O2N) 2C(CH2CH2CO2Me) 2, instead of the expected adduct (Klager, CA 53, 6060c). Similar behavior was noted with I (R = NO2, CN). Apparently II underwent a reverse Mannich reaction to give the anion, HOCH2C(NO2): NO2-(III). Gradual acidification of the K salt of III with dilute H2SO4 to pH 4 gave KO2N:C(NO2)CH2C(NO2):NO2K, apparently via formation of H2C:C(NO2)2 as an intermediate. The Mannich reaction of polynitro-1,5-pentanediols with amines gave cyclic derivs., whereas similar reactions of 2,2-dinitro-1,3-propanediol gave the linear products in some instances and cyclic derivs. in others; the latter appear to result from in situ formation of the anion of HOCH2C(NO2)2CH2CH(NO2)2.

L16 ANSWER 34 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1962:455645 HCAPLUS

DOCUMENT NUMBER: 57:55645

ORIGINAL REFERENCE NO.: 57:10992i,10993a-f

TITLE: Polynitro aliphatic nitramines
AUTHOR(S): Frankel, Milton B.; Klager, Karl
CORPORATE SOURCE: Aerojet-Gen. Corp., Azusa, CA

SOURCE: Journal of Chemical and Engineering Data (1962)

), 7, 412-13

CODEN: JCEAAX; ISSN: 0021-9568

DOCUMENT TYPE: Journal LANGUAGE: Unavailable

The Mannich condensation of 2,2-dinitro-1-alkanols with NH3 was extended to include polynitro aliphatic primary amines and diamines, which were prepared by acid hydrolysis of the corresponding isocyanates. Nitration of the secondary amines thus obtained gave the corresponding nitramines, which were sensitive to impact. To 23.1 g. (O2N)3CCH2CH2NH2.HCl (I.HCl), 18.1 g. (O2N)3CCH2OH (II), and 150 mL. H2O was added dropwise 88 mL. 1.136N NaOH at room temperature with stirring and the mixture cooled in an ice bath to give 28.2 g. (O2N)3CCH2NHCH2CH2C(NO2)3 (IIa), m. 64-5° (CHCl3). The following Mannich condensation products were prepared similarly (alc., amine, product, % yield, m.p. given): II, MeC(NO2)2CH2NH2 (III), MeC(NO2)2CH2CH2NHCH2C(NO2)3, 71.7, oil; MeC(NO2)2CH2OH (IV), I, MeC(NO2)2CH2NHCH2CH2C(NO2)3, quant., oil; (O2N)2C(CH2OH)2 (V), III, (O2N) 2C[CH2NHCH2CH2C(NO2) 2Me] 2, 74.2, 95-110°; V, I, (O2N) 2C [CH2NHCH2CH2C(NO2)3]2, 83.8, 70-80°; II, CH2(NH2)2, CH2[NHCH2C(NO2)3]2, 93.1, 100.5°; IV, (O2N)2C(CH2CH2NH2)2 (VI), (O2N) 2C[CH2CH2NHCH2C(NO2) 2Me] 2, quant., oil; II, VI, (O2N) 2C[CH2CH2NHCH2C(NO2)3]2, 65.7, 93-5°; II, O2NN(CH2CH2NH2)3, O2NN [CH2CH2NHCH2C (NO2) 3] 2, 33.1, qum; II, [H2NCH2CH2N (NO2) CH2] 2, [(O2N)3CCH2NHCH2CH2N(NO2)CH2]2, quant., 100-5°; II, O2NN [CH2C (NO2) 2CH2CH2NH2] 2, O2NN [CH2C (NO2) 2CH2CH2NHCH2C (NO2) 3] 2, 31.3, 90-100°. Com. absolute HNO3 (150 mL.) cooled in an ice bath, treated

mL.

dropwise with 150 mL. Ac20 at below 5-10° followed by 28.2 g. IIa, the mixture warmed to 30° to effect solution (in some cases the amine dissolved at 5-10° and it was unnecessary to raise the temperature), and the solution poured on ice gave 27.0 g. (O2N)3CCH2N(NO2)CH2CH2C(NO2)3, m. 144-5° (CHCl3). To 53.0 g. VI.2HCl, 60 g. IV, and 400 mL. H2O was added dropwise 82 mL. 4.877N NaOH, the aqueous layer decanted from a solid which separated, the solid dried, treated with 200 mL. concentrated H2SO4-300

tech. 100% HNO3, the mixture warmed 20 min. at 50-5°, cooled, and the precipitate (80 g.) filtered off (an addnl. 6.0 g. was obtained by pouring the filtrate on ice) gave (O2N)2C[CH2CH2N(NO2)CH2C(NO2)2Me]2, m. 206-8° (Me2CO). The following compds. were prepared by these procedures (product, % yield, m.p., recrystn. solvent given): MeC(NO2)2CH2CH2N(NO2)CH2C(NO2)3, 38.3, 105-7°, CHCl3; MeC(NO2)2CH2N(NO2)CH2CH2C(NO2)3, 63.3, 109-9.5°, CCl4; (O2N)2C[CH2N(NO2)CH2CH2C(NO2)2Me]2, 61.2, 137-9°, (ClCH2)2 (VII); (O2N)2C[CH2N(NO)CH2CH2C(NO2)2Me]2, 67.2, 124-5°, VII; (O2N)2C[CH2N(NO2)CH2CH2C(NO2)3]2, 50.0, 157-9°, MeOH-H2O, CH2[N(NO2)CH2C(NO2)3]2, 20.0, 84-5°, cyclohexane; (O2N)2C[CH2CH2N(NO2)CH2C(NO2)3]2, 69.8, 170-5°, 100% HNO3; O2NN[CH2CH2N(NO2)CH2C(NO2)3]2, 45.1, 166-7°, 70% HNO3; O2NN[CH2C(NO2)2CH2CH2N(NO2)CH2C(NO2)3]2, 45.1, 166-7°, MeNO2-CCl4.

L16 ANSWER 35 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1962:442520 HCAPLUS

DOCUMENT NUMBER: 57:42520

ORIGINAL REFERENCE NO.: 57:8432e-i,8433a-b

TITLE: Dinitroacetonitrile. III. Dinitroacetamide and its

derivatives

AUTHOR(S): Parker, Charles O.

CORPORATE SOURCE: Rohm & Haas Co., Huntsville, AL SOURCE: Tetrahedron (1962), 17, 105-8 CODEN: TETRAB; ISSN: 0040-4020

DOCUMENT TYPE: Journal LANGUAGE: Unavailable

AB Manipulation of preparative quantities of (O2N)2CHCONH2 (I) or its salts was troublesome due to unfavorable solubility properties and relatively facile decomposition to (O2N)2CH2 derivs. Anhydrous Et2O (200 ml.) stirred at -5° (ice-Me2CHOH bath) with passage of dry HCl under anhydrous conditions, the saturated solution treated rapidly with 15.3 g. dried NaC(O2N)2CN in 24 ml. 1:1 anhydrous MeOH-EtOAc with rise of temperature to 4-5°, the mixture kept 16 hrs. at -10° (freezing mixture in Dewar flask), filtered through Celite, the solvent removed in vacuo, and the product washed with CH2Cl2 yielded 76-5% I, m. 86-7°. Concentrated HCl (83 ml.) stirred at -10° with portionwise addition of NaC(NO2)2CN, the temperature raised to 20° in 16 hrs., filtered through Celite, and the filtrate extracted continuously with 800 ml. CH2Cl2 yielded 14.7% I. The filtrate from a similar run diluted with 83 ml. H2O, extracted 3 times with 85 ml. (Me2CH)2O, the extract dried over anhydrous Na2SO4 and anhydrous MgSO4, and the dried filtered

solution evaporated yielded 14.1% I, m. $48-67^{\circ}$ (CH2Cl2). I (24.2 g.) in 20 ml. H2O stirred with dropwise addition of 13.5 ml. formalin, kept 16 hrs. at 20° saturated with NaCl, and extracted with Et2O yielded 39.4% H2NCO(O2N)2CCH2OH (II), m. $104-7^{\circ}$, v 1710, 1575 cm.-1 (CF3CO)2O (14 g.) and 3.4 g. HCOH refluxed 15 min., the cooled solution stirred with addition of 10.1 g. II in 50 ml. Et2O, refluxed 1.5 hrs., freed from solvent, the residue taken up in CH2Cl2, the solution extracted twice with H2O, twice with

aqueous NaHCO3, and again with H2O, the dried solution concentrated, and the chilled

5%

concentrate diluted with petr. ether gave 1.5 g. product, m. 55-8°, recrystd. from CH2Cl2-petr. ether to give H2NCO(O2N)2CCH2OAc, m. 60-2°. Freshly crystallized MeCH: CHCONH2 (1.7 g.) and 0.6 g. paraformaldehyde ground in a mortar, the mixture triturated with 2 drops of saturated aqueous K2CO3, warmed several min. at 60°, the clear solution taken up in 10 ml. H2O, the filtered solution warmed 10 min. at 60° with 3 $\,$ g. I, and filtered yielded 18.3% product, m. 116-17°, recrystd. front ClCH2CH2Cl to give MeCH: CHCONHCH2C(NO2) CONH2, m. 120°. I(3.0g.)in 7ml. H2O kept 16 hrs. at 20° with 1.4 g. H2C:CHCO2H and the volatile material evaporated in vacuo gave 2.8 g. CH2Cl2-washed material, m. $80-95^{\circ}$, recrystd. from C2H4Cl2 to give H2NCO(O2N)2CCH2CH2OC2 m. 115-17°. H2C:CHCONH2 (1.4 g.) in 5 ml. MeOH and 3.0 q. I in 10 ml. MeOH warmed 16 hrs. at 40°, the filtered solution evapd, in vacuo, the residue diluted with cold H2O, and the dried product (2.7 g., m. 105-6°) recrystd. from C2H4Cl2 gave H2NCO(O2N)2CCH2CH2CONH2, m. 110-11°. I (5 g.) in 10 ml. MeOH stirred with cooling (ice bath) and dropwise addition of NaOH-MeOH until faintly alkaline gave 5.2 g. salt, m. 167° (decomposition), recrystd. from alc. Et20 to give I Na salt, m. 170° (with explosion). Similarly were prepared the corresponding K and Ag salts, m. 159, and 130° resp.

L16 ANSWER 36 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

1962:435929 HCAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 57:35929 ORIGINAL REFERENCE NO.: 57:7106c-f

TITLE: Aliphatic nitrazapolynitro diamines INVENTOR (S): Frankel, Milton B.; Klager, Karl

PATENT ASSIGNEE(S): Aerojet-General Corp.

SOURCE: 2 pp. DOCUMENT TYPE: Patent LANGUAGE: Unavailable

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE -----------------**--**---US 3000950 19610919 US

19570304 <--AB Diamines useful as high explosives were obtained by condensing suitable diammonium salts with 2,2,2-trinitroethanol (I) at pH 4-8. A solution of 6.46 g. I, followed by 1.34 g. NaOH in 10 ml. H2O, was added to a solution of 9.1 g. 3,3,5,7,7-pentanitro-5-aza-1,9-nonanediammouium dinitrate at 48°. The mixture was stirred 30 min. and chilled while standing over night, giving yellow 1,1,1,6,6,8,10,10,15,15,15-undecanitro-3,8,13triazapentadecane, m. 90-105° (decomposition). U.S. 3,000,951, Appl. Mar. 7, 1957; 2 pp. The nitration of the diamines of the preceding patent yields nitramines which are high explosives. 1,1,1,6,6,11,11,11-Octanitro-4,8-diazaundecane was added to a solution of 40 ml. 100% HNO3 and 40 ml. Ac20 at 5°, the solution warmed to room temperature and poured on ice, the precipitate washed with H2O, dried, and recrystd. from HNO3, giving 1,1,1,4,6,6,8,11,11,11-decanitro-4,8-diazaundecane, m. 135-7°, impact stability 10-15 cm./2 kg., heat of combustion 1984 cal./g., lead block and ballistic mortar values 177 and 155, resp. (TNT = 100). Also prepared was 2,2,5,7,7,9,12,12-octanitro-5,9-diazatridecane, m. 137-9°, heat of combustion 2897 cal./g., lead block and ballistic mortar values 128 and 140, resp. (TNT = 100).

L16 ANSWER 37 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

1962:24732 HCAPLUS

ACCESSION NUMBER: DOCUMENT NUMBER: 56:24732 ORIGINAL REFERENCE NO.: 56:4619a-b

TITLE: Nitroparaffins INVENTOR(S): Urushibara, Shozo

DOCUMENT TYPE: Patent LANGUAGE: Unavailable

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

JP 36010314 B4 19610000 JP 19581002 <--

AR A lower hydrocarbon was treated with HNO3 in the gas phase in the presence of O (air, or halogen) and a radical formation accelerator selected from di-tertbutyl peroxide, azobisisobutyronitrile, benzoyl peroxide, or alkali bichromate.

L16 ANSWER 38 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1961:84337 HCAPLUS DOCUMENT NUMBER: 55:84337

ORIGINAL REFERENCE NO.: 55:15934c-e

TITLE: Nitrate salts of aliphatic polynitro amines INVENTOR(S): Frankel Milton P

PATENT ASSIGNEE(S): Aerojet-General Corp.

DOCUMENT TYPE: Patent

LANGUAGE: Unavailable

LANGUAGE: Unavailable

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE 19610404 US -----US 2978509

AB The title compds., used as explosives or as O donors in propellants, are prepared by treating an isocyanate with HNO3. For example, MeC(NO2)2(CH2)2NCO was refluxed on a steam bath with a 10-fold excess of 35% HNO3 for 3 hrs. The solution was evaporated to dryness in vacuo, and the quant. yield of MeC(NO2)2(CH2)2NH2.HNO3 recrystd. from EtOAc and Et2O, m. 130-3°; Pb block value, 112, TNT = 100; ballistic mortar value, 116, TNT = 100. Similarly, C(NO2)3(CH2)2NH2.HNO3 was prepared from the related isocyanate. Cf. U.S. 2,978,511 (2nd following abstract).

L16 ANSWER 39 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1961:84336 HCAPLUS DOCUMENT NUMBER: 55:84336 ORIGINAL REFERENCE NO.: 55:15934b-c

Symmetrical secondary aliphatic polynitro diamines

PATENT ASSIGNEE(S): Aerojet-General Corp.
DOCUMENT TYPE: Patent
LANGUAGE:

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE
US 2978508 19610404 US

The diamines, used as explosives, are prepared by condensing a geminal polynitro-containing amine with C(NO2)2[CH2OH]2 (I). For example, 88 ml. of 1.136N NaOH was added to 0.05 mole I and 0.10 mole C(NO2)3(CH2)2NH2.HCl in 50 ml. H2O. The yellow precipitate of C(NO2)2[CH2NH(CH2)2C(NO2)3]2 was washed with H2O and dried to give an 88% yield of a tan solid, m. 70-80°

with decomposition; Pb block value, 143, TNT = 100, ballistic mortar value, 146, TNT = 100. C(NO2) 2 [CH2NH(CH2) 2C(NO2) 2Me] 2 was prepared in like manner from the related amine. Cf. U.S. 2,978,505, 2,978,506, 2,978,507, and 2,978,512 (preceding and following abstrs.).

L16 ANSWER 40 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1957:12975 HCAPLUS

DOCUMENT NUMBER: 51:12975

ORIGINAL REFERENCE NO.: 51:2814g-i,2815a-i,2816a

TITLE: Derivatives of 4,5-dihydronaphtho [1,2]

thiazole-2-thiol and -s-triazines

AUTHOR(S): D'Amico, John J.; Harman, Marion W.

CORPORATE SOURCE: Monsanto Chem. Co., Nitro, WV

SOURCE: Journal of the American Chemical Society (1956

), 78, 5345-8

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 51:12975
GI For diagram(s), see printed CA Issue.

AB H2NCS2NH4 (330 g.) and 1500 cc. EtOH treated with stirring with 642 g. 2-bromo-1-tetralone, the mixture stirred 18 hrs., heated 2 hrs. at 75-8°, cooled to 10°, and filtered, and the residue washed with H2O and air-dried yielded 80.5 g. 4,5-dihydronaphtho[1,2]thiazole-2-thiol (I), tan solid, m. 206-8° (from EtOH). I (25 g.) in 200 cc. H2O treated dropwise with stirring with 28.6 g. (NH4)2S2O8 in 70 cc. H2O during 40 min. at 25-30°, and the mixture stirred 2 hrs. and filtered yielded 96.5% 2,2'-dithiobis(4,5-dihydronaphtho[1,2]thiazole), tan solid, m. 125-6° (from EtOH). I (43.9 g.), 11.2 g. KOH, and 600 cc. Me2CO treated dropwise with stirring at 20° with 30.3 g. Et2NCSCl in 150 cc. Me2CO, the mixture stirred 5 hrs. and filtered, the filtrate added to 700 g. ice water and stirred 15 min., and the solid precipitate isolated yielded

98.5% 4,5-dihydronaphtho[1,2]thiazol-2-yl diethyldithiocarbamate, tan solid, m. 117-18° (from EtOH). Iodine (32.4 g.) and 34.8 g. KI in 420 cc. H2O added dropwise at 25-30° during 1.5 hrs. with stirring to 24 g. I, 35.2 g. 25% aqueous NaOH, 100 g. H2O, and 108.9 g. cyclohexylamine, the mixture stirred 1 hr. and extracted with Et2O, and the extract

worked up yielded 86% N-cyclohexyl-4,5-dihydronaphtho[1,2]thiazole-2sulfenamide, m. 74-6° (from EtOH). Benzoquinone (27 g.) and 185 cc. MeOH heated to 50°, the solution cooled to 0° and treated with 54.9 g. I and 300 cc. MeOH in 1 portion, the mixture stirred 2 hrs. at 5-10°, heated to 60°, added to 1000 cc. hot H2O, stirred 0.5 hr., and filtered, and the residue washed with 500 cc. hot H2O and air-dried at 50° yielded 90.5% (4,5-dihydronaphtho[1,2]thiazol-2ylthio)hydroquinone, m. 236-8° (from CHCl3). I (20 g.), 300 cc. Me2CO, and 5.1 g. KOH treated dropwise with 5.6 g. cyanuric chloride (II) in 400 cc. Me2CO, heated 5 hrs. at 50-5°, cooled to 25°, and filtered yielded 98.5% 2,4,6-tris(4,5-dihydronaphtho[1,2]thiazol-2-ylthio)s-triazine, m. 238-9° (from C6H6). ZnCl2 (6.2 g.) in 100 cc. H2O added with stirring to 20 g. I, 14.6 g. 25% aqueous NaOH, and 2000 cc. H2O at 80°, the mixture stirred 2 hrs. without heating, and the solid filtered off gave 99% Zn salt of I, m. 180-90° (decomposition). 2,4-(O2N)2C6H3Cl (20.3 g.) added in 1 portion with stirring to 21.9 g. I, 5.6 g. KOH, and 300 cc. Me2CO, the mixture stirred 5 hrs. at 50-6°, cooled to room temperature, poured onto 700 g. crushed ice, stirred 1 hr., and filtered, and the residue washed and dried at 50° yielded 80.5% 2-(2,4-dinitrophenylthio)-4,5-dihydronaphtho[1,2]thiazole, m.

173-4° (from EtOAc). I (54.9 g.), 40 g. 25% aqueous NaOH, and 500 cc. H2O treated with stirring with 36 g. Me2N(CH2)2Cl.HCl and 40 g. 25% aqueous NaOH, the mixture heated 5 hrs. with stirring at 50-60°, cooled to 25°, and extracted with Et2O, and the extract worked up gave 82.5% 4,5-dihydro-2-(2-dimethylaminoethylthio)naphtho[1,2]thiazole, amber oil. I (43.8 g.) treated with 11.2 g. KOH in 500 cc. Me2CO, the solution treated at room temperature with 12.3 g. (.tplbond.CCH2Cl)2, the mixture heated 24 hrs. at

50-6°, poured onto 500 g. crushed ice, stirred 10 min., and filtered, and the residue washed and dried gave 98.2% 2,2'-(2-butynylenedithio)bis(4,5-dihydronaphtho[1,2]thiazole) (III), m. 145-6° (from EtOAc). A similar run using 12.5 g. (:CHCH2Cl)2 gave 98.5% 2-butenylenedithio analog of III, m. 113-14° (from EtOH). I (109.6 g.), 500 cc. H2O, and 80 g. 25% aqueous NaOH treated with stirring with 44.8 g. MeCHClCN, the mixture heated 2 hrs. at 50-60°, kept 3 hrs. at 25-30°, diluted with stirring with 400 cc. Et2O, stirred 15 min., and filtered, and the residue dried gave 56 g. unchanged I; the filtrate washed with H2O, dried, and distilled gave 85.2% (38.3% conversion) 3-(4,5-dihydronaphtho[1,2]thiazol-2-ylthio)propionitrile, amber oil. I (33 g.), 8.4 g. KOH, and 300 cc. Me2CO treated with stirring with 20.2 g. Ac2CHCl in 1 portion, the mixture stirred 5 hrs. and filtered, the filtrate poured onto 500 g. crushed ice and stirred 20 min., and the precipitate filtered.

washed, and dried yielded 90.5% 3-(4,5-dihydronaphtho[1,2]thiazol-2ylthio)-2,4-pentanedione, m. 105-6° (from EtOH). A similar run with 14 g. ClCH2Ac gave 91.1% 2-(acetonylthio)-4,5dihydronaphtho[1,2]thiazole, m. 68-9° (from EtOH). A similar run with 24.8 g. AcCHClCO2Et filtered, the Me2CO filtrate evaporated in vacuo, the residue dissolved in 500 cc. Et20, and the Et20 solution worked up gave 90.3% Et α -(4,5-dihydronaphtho [1,2]thiazol-2-ylthio)acetoacetate, oil. (21.9 g.), 5.6 g. KOH, and 300 cc. Me2CO treated with stirring with 0.1 $\,$ mole CH2: CHCH2Cl, and the mixture heated 5 hrs. at 55-6°, filtered, and evaporated in vacuo up to 90° gave 96.5% 2-allylthio-4,5dihydronaphtho[1,2]thiazole (IV), oil. A similar run with 0.1 mole C1CH2CH:CClMe carried out in the same manner, the filtrate poured onto 500 g. crushed ice, stirred 15 min., and filtered, and the residue washed and dried gave 88.0% 2-(MeCCl:CHCH2) analog of IV, m. 63-5°. ClCH2CCl:CH2 (0.1 mole) gave similarly 98.7% 2-(CH2:CClCH2) analog of IV, m. 60-1° (from EtOH). Na, K, or amine salt (1 mole) of the appropriate dialkyldithiocarbamic acid dissolved in 1000 cc. Me2CO at 56°, the solution treated dropwise with stirring with 61.5 g. II in 500 cc. Me2CO, the mixture heated 4 hrs. with stirring at 55-6° and filtered at 55-6°, the filtrate concentrated in vacuo to 100 cc. and diluted with stirring with 200 cc. heptane, and the mixture stirred 20 min., and filtered yielded the corresponding I compound RC:N.CR':N.CR':N (R, R', m.p., % crude yield, and dialkyldithiocarbamic acid salt used are given): Me2N, Me2NCS2, 172-3° (from dioxane), 48.0, Me2NCS2Na; Et2NCS2, Et2NCS2, 136-7°, 39.5, Et2NCS2K; iso-Pr2NCS2, iso-Pr2NCS2, 119-20° (from dioxane), 31.4, iso-Pr2CS2K; Me2N, Me2NCS, 163-4° (from C6H6), 84.3, Me2NCS2NH2Me2; Et2N, Et2NCS2, 115-16° (from EtOH), 56.9, Et2NCS2NH2Et2; iso-Pr2N, iso-Pr2NCS2, 218° (from dioxane), 39.9, iso-Pr2NCS2NH2(CHMe2)2.

L16 ANSWER 41 OF 41 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1957:12974 HCAPLUS

DOCUMENT NUMBER: 51:12974
ORIGINAL REFERENCE NO.: 51:2814a-g

TITLE: Derivatives of 4-nitrazapentanonitrile AUTHOR(S): Frankel, Milton B.; Klager, Karl

10604774.trn Page 50

SOURCE:

Journal of the American Chemical Society (1956

), 78, 5428-30

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE:

Journal

LANGUAGE: Unavailable

AB 4-Azapentanonitrile (I) (1260 g.) added with stirring to 1485 g. 70% HNO3 at 0-5° and filtered yielded 1200 g. I.HNO3, m. 70-1°. Concentrated HCl (13.8 cc.) and 42 cc. tech. grade 100% HNO3 added successively dropwise with stirring to 840 cc. Ac2O, the mixture treated at 20-5° with 735 g. I.HNO3 in portions during 0.5 hr., warmed to 30°, stirred 2 hrs., cooled to 5° and diluted with 2 l. ice water, the aqueous phase extracted with 600 cc. CH2Cl2, and the combined oily layer and CH2Cl2 extract worked up yielded 600 g. 4-nitrazapentanonitrile (II), light yellow liquid, b0.040 60-70°, n25D 1.4863. Dry HCl bubbled, with stirring, into 129.0 g. II, 130 cc. MeOH, and 130 cc. absolute Et20 to saturation,

the mixture stirred 2.5 hrs. at 0-5° and filtered, the white solid filter residue added to 130 cc. H2O, neutralized with saturated aqueous NaHCO3

heated 0.5 hr. at 50°, the aqueous phase extracted with CH2Cl2, and the combined oily layer and CH2Cl2 extract worked up gave 100 g. Me ester (III) of 4-nitrazapentanoic acid (IV), colorless liquid, b1 107°, n25D 1.4694; similarly was prepared the Et ester of IV, b1 112°, n25D 1.4644. II (812 g.) and 2436 cc. concentrated HCl heated 8 hrs. on the steam bath, cooled, and extracted with CH2Cl2, and the extract worked up gave 463.5

IV, white solid, m. 53-4° [from (CH2Cl)2]. III (162.0 g.) and 325 cc. concentrated HCl refluxed 3 hrs. and concentrated in vacuo yielded 102.0 g. IV, m.

53-4° (from iso-Pr2O). IV (148 g.) added portionwise to 240 cc. SOC12, warmed gently on the steam bath to initiate the reaction, refluxed 2 hrs., cooled, and concentrated gave 100% crude chloride (V) of IV, light yellow liquid, b0.010 100-7°, n25D 1.4997. (CH2OH)2 (12:0 g.), 84.0 g. V, and 200 cc. CHCl3 refluxed 20 hrs., cooled, washed, and worked up yielded 43.0 g. ethylene bis-4-nitrazapentanoate, white solid, m. 58-8.5° (from MeOH). V (167.0 g.) in 150 cc. CHCl3 added slowly with stirring to 130.0 g. NaN3 in 390 cc. H2O at 10-15°, and stirred 0.5 hr. at 10°, the aqueous layer extracted with 150 cc. CHCl3, the extract washed, dried, filtered, and refluxed until the N evolution ceased, and the solution concentrated in vacuo gave 133 g. 3-nitrazabutyl isocyanate (VI),

white crystals, m. 25-6° (from dry Et20). VI (29.0 g.) and 30 cc. MeOH refluxed 0.5 hr. and concentrated in vacuo gave 30.1 g. Me 3-nitrazabutylcarbamate, white solid, m. 87-8° (from CHCl3-CCl4). VI (29.0 g.) treated with 50 cc. 35% HNO3, warmed 1 hr. on the steam bath, and concentrated in vacuo yielded 3-nitrazabutylammonium nitrate, white needles,

m. 120-1° (from MeOH). Concentrated HCl and VI gave similarly the chloride analog, m. 132-3°. 3-Nitrazabutylamine (VII) (11.9 g.) in 50 cc. CHCl3 treated with 7.3 g. (CO2Et)2 yielded 9.9 g. N,N'-bis(3-nitrazabutyl) oxamide (VIII), white solid, m. 225-30°. VIII (9.0 g.), 140 cc. 100% HNO3, and 130 cc. concentrated HCl heated with stirring 35 min. at 50-5°, cooled, and poured onto ice yielded 8.8 g. di-NO2 derivative, m. 168-9° (from Me2CO). VII.HCl (15.6 q.), 25 cc. H2O, and 8.1 g. 37% aqueous CH2O treated dropwise with 8.2 g. NaOAc in 15 cc. H2O, stirred 0.5 hr., and filtered yielded 5.9 q. 1,3,5-tris(3nitrazabutyl)hexahydro-1,3,5-triazine, m. 97-7.5° (from EtOAc). VII.HCl (46.5 g.), 24.9 g. (O2N) 2C(CH2OH) 2, and 100 cc. H2O treated dropwise with 24.6 g. NaOAc in 75 cc. H2O and filtered gave 34.6 g. 2,7,7,

12-tetranitro-2,5,9,12-tetraazatridecane (IX), yellow solid, m. 110-15°. IX (3.68 g.), 0.81 g. 37% aqueous CH2O, and 100 cc. H2O stirred 1 hr. at room temperature and 1 hr. at 40-5° yielded 3.2 g. 1,3-bis(3-nitrazabutyl)-5,5-dinitrohexahydro-1,3-diazine, tan solid, m. 120-1° (from CHCl3).

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L19 ANSWER 1 OF 20 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2005:168855 HCAPLUS

DOCUMENT NUMBER: 143:221244

TITLE: Multidentate aminoalkoxides. Synthesis and

complexation behavior to lithium and sodium

AUTHOR(S): Mueller, Gerhard; Schaetzle, Torsten

CORPORATE SOURCE: Fachbereich Chemie, Universitaet Konstanz, Konstanz,

D-78464, Germany

SOURCE: Zeitschrift fuer Naturforschung, B: Chemical Sciences

(2004), 59(11/12), 1400-1410 CODEN: ZNBSEN; ISSN: 0932-0776

PUBLISHER: Verlag der Zeitschrift fuer Naturforschung

DOCUMENT TYPE: Journal LANGUAGE: English

The tris(dimethylaminomethyl)-substituted alc. (R2NCH2)3COH (R = Me, 1) was synthesized by reaction of 1-chloro-2,3-epoxy-2-chloromethylpropane with a large excess of 40% aqueous HNMe2 in 95% yield as colorless liquid (b.p. 87°/1 mbar). Similar syntheses led to the resp. amino alcs. with R = Et, CH2Ph. The dimethylamino alc. 1 was characterized crystallog. as the trihydrochloride salt 2. Reaction of 1 with elemental sodium in toluene gave the tetrameric alcoholate [(Me2NCH2)3CONa]4 (3) which has a heterocubane structure in the solid state. In addition to three oxygen atoms, each sodium atom is coordinated by two amino groups from two different adjacent ligands (Na-N 2.529(3)/2.628(3) Å). Reaction of 1 with LiNMe2 afforded the lithium alcoholate which crystallized as dimeric mixed-anion aggregate [(Me2NCH2)3COLi·LiNMe2]2 (4). It has a four-rung ladder structure consisting of two four-membered Li(NMe2)LiO rings connected through a central LiOLiO ring. All ligand amino groups are lithium-coordinated (Li-N 2.117(6)/2.101(6)/2.218(6) \mathring{A}) as is the amido nitrogen atom (Li-N 1.964(6)/2.027(6) Å). Reaction of 1 with LitBu in n-hexane also led to deprotonation at oxygen. In one ligand one Me group is deprotonated, in a 2nd one two Me groups are lithiated leading to doubly and triply charged anions, resp. The product crystallizes as the dimeric mixed-anion aggregate [(-H2CN(Me)CH2)(Me2NCH2)2CO-·5Li+·(-H2CN(Me)CH2)2(Me2NCH2)CO-]2 (5) having a core of 10

Li+ cations, 4 alcoholate oxygen atoms, and 6 N(Me)-CH2- groups.

REFERENCE COUNT: 97 THERE ARE 97 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 2 OF 20 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2005:29032 HCAPLUS

DOCUMENT NUMBER: 142:114074

TITLE: Preparation of polyazido carboxylic acid esters
INVENTOR(S): Dave, Paritosh R. Duddu, Raja G.; Damavarapu, Reddy;
Celber Nathaniel; Yang, Kathy; Surapaneni, C. Rao

PATENT ASSIGNEE(S): (United States Dept. of the Army, USA

SOURCE: U.S., 9 pp.

CODEN: USXXAM

DOCUMENT TYPE: Patent LANGUAGE: English

10604774.trn Page 52 10:44

FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 6841690 US 6965042 PRIORITY APPLN. INFO.:	B1 B1	20050111	US 2003-604778 US 2003-604777 US 2002-319801P	 P	20030815 20030815 20021219

Y X
$$III$$
 III III III III III III III

AB This invention relates to a series of novel compds., such as I = N3, OH, ONO2, NO2; Y = CH2N3, NO2; A, B = N3, 4-carboxytriazolomethyl], and II [Z = CH2, O, NOH, 2,4-dihydrophenylhydrozono], including 2-azido-2-azidomethyl-1,3-diazidopropane, 2-azidomethyl-2-hydroxy-1,3diazidopropane, 2-azidomethyl-2-nitrato-1,3-diazidopropane, 2-azidomethyl-2-nitro-1,3-diazidopropane, 2,2-dinitro-1,3-diazidopropane, methallyidiazide, a dimer of methallyidiazide, comprising 3a,8a-bis-azidomethyl-3a,4,8a,9-tetrahydro-3H,8H-bis[1,2,3]triazolo[1,5-a; 1'',5''-d]pyrazine, 1,3-diazidoacetone, and 2-oximido-1,3-diazidopropane. Also shown are reaction intermediates of these compds., including 2,2-bis(chloromethyl)oxirane, and 2,2-bis(azidomethyl)oxirane. In addition, a number of potentially useful energetic compds. have been prepared from the low mol. weight polyazido compds. above, including N-2(azido-1-azidomethylethylidene) -N''-(2,4-dinitrophenyl) -hydrazine (7-DNPH), 1,3-bis(4-carboxytriazolyl)2,2-dinitropropane, tris(4carboxytriazolomethyl)methanol, benzene-1,3,5-tricarboxylic acid tris(2-azido-1,1-bisazidomethyl-ethyl)ester, adamantane 1,3,5,7-tetracarboxylic acid tetrakis(2-azido-1,1-bisazidomethy1ethyl)ester, adamantane carboxylic acid (2-azido-1,1-bisazidomethylethyl)ester, cubane 1,3,5,7-tetracarboxylic acid tetrakis (2-azido-1,1-bisazidomethyl-ethyl)ester, cubane 1,4-dicarboxylic acid bis(2-azido-1,1-bisazidomethyl-ethyl)ester. Thus, tris(4carboxytriazolomethyl)methanol (III) was prepared by the reaction of 2-azidomethyl-2-hydroxy-1,3-diazidopropane I [A, B = N3; X = CH2N3; Y = OH] (also prepared) with propiolic acid. REFERENCE COUNT: THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS

L19 ANSWER 3 OF 20 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:884285 HCAPLUS

DOCUMENT NUMBER: 142:355291

TITLE: Preparation of multi-aza-C60 derivatives

INVENTOR(S): Chen, Xiaolian; Tang, Guangshi

PATENT ASSIGNEE(S): Peop. Rep. China

10604774.trn

Page 53

10:44

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

SOURCE: Faming Zhuanli Shenqing Gongkai Shuomingshu, 8 pp.

CODEN: CNXXEV

DOCUMENT TYPE: Patent LANGUAGE: Chinese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. --------------CN 2002-121196 CN 2002-121196 CN 1465576 Α 20040107 20020611 PRIORITY APPLN. INFO.: The method comprises cycloaddn. of C60 with multi-triazo compound, e.g.

2-methyl-2-nitro-1,3-di(triazo)propane, in organic solvent, such as toluene, chlorobenzene, xylene, etc., and purification on 200-300 mesh silica gel column with toluene-petroleum ether (3-5:3-5, volume/volume) as eluent.

L19 ANSWER 4 OF 20 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:807738 HCAPLUS

DOCUMENT NUMBER: 142:6481

TITLE: The First Trisaza-Bridged [60] Fulleroid: Drilling a

Hole on the Fullerene

Tang, Guang-Shi; Chen, Xiao-Lian; Zhang, Sheng-Yuan; AUTHOR (S):

Wang, Jing

CORPORATE SOURCE: Key Laboratory of Science and Technology of

Controllable Chemical Reactions, Ministry of

Education, Beijing University of Chemical Technology,

Beijing, 100029, Peop. Rep. China

SOURCE: Organic Letters (2004), 6(22), 3925-3928

CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

Journal . DOCUMENT TYPE: English LANGUAGE:

OTHER SOURCE(S): CASREACT 142:6481

Two types of trisaza-bridged [60] fulleroids have been synthesized. means of 13C NMR, 1H NMR, MALDI-TOF MS, FTIR, UV-vis, and 2D-NMR (gHSQC,

gHMBC, and NOSEY) spectroscopy, they have been shown to be

tris[6,5]-opened-aza-bridged adducts with substituents on the same five-membered ring with Cs symmetry. Some data of nonlinear optics and

electrochem. for the product are also reported.

REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 5 OF 20 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:717422 HCAPLUS

DOCUMENT NUMBER: 141:366573

TITLE: Click chemistry in materials synthesis. 1. Adhesive

polymers from copper-catalyzed azide-alkyne

cycloaddition

AUTHOR (S): Diaz, David D.; Punna, Sreenivas; Holzer, Philipp;

McPherson, Andrew K.; Sharpless, K. Barry; Fokin,

Valery V.; Finn, M. G.

Department of Chemistry, The Scripps Research CORPORATE SOURCE:

Institute, La Jolla, CA, 92037, USA

Journal of Polymer Science, Part A: Polymer Chemistry SOURCE:

(2004), 42(17), 4392-4403

CODEN: JPACEC; ISSN: 0887-624X

PUBLISHER: John Wiley & Sons, Inc.

DOCUMENT TYPE: Journal English LANGUAGE:

10604774.trn Page 54 10:44

AB The copper(I)-catalyzed cycloaddn. reaction between azides and alkynes has been employed to make metal-adhesive materials. Copper and brass surfaces supply the necessary catalytic Cu ions, and thus the polymerization process occurs selectively on these metals in the absence of added catalysts. Alternatively, copper compds. can be added to monomer mixts. and then introduced to reducing metal surfaces such as zinc to initiate polymerization The resulting materials were found to possess comparable or superior adhesive strength to standard com. glues, and structure-activity correlations have identified several important properties of the monomers.

REFERENCE COUNT:

40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 6 OF 20 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

2004:137939 HCAPLUS

DOCUMENT NUMBER:

140:357709

TITLE:

Preparation of cage molecule based polyazido core

units for dendrimer synthesis

AUTHOR (S):

Dave, Paritosh R: Duddu, Raja; Yang, Kathy;

Damavarapu, Reddy; Gelber, Nathaniel; Surapaneni, Rao;

Gilardi, Richard

CORPORATE SOURCE:

GEO-CENTERS, INC. at ARDEC, Picatinny Arsenal, NJ,

07806-5000, USA

SOURCE:

Tetrahedron Letters (2004) 45 (10), 2159-2162

CODEN: TELEAY; ISSN: 0040-4039 Elsevier Science B.V.

PUBLISHER:

DOCUMENT TYPE:

Journal

LANGUAGE:

English

Core mols. based on benzene-, cubane-, and adamantane-polycarboxylates with peripheral polyazido substitution were prepared The first synthesis of 1,3-diazidoacetone and its conversion to the corresponding oxime, DNPH, and 2,2-dinitro derivs. is also reported. All azido compds. should be considered dangerous and proper precautions should be taken during handling and storage of these mols.

REFERENCE COUNT:

THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS 17 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 7 OF 20 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

2002:605702 HCAPLUS

DOCUMENT NUMBER:

138:75615

TITLE:

Novel polyazido/polynitrato compounds derived from

AUTHOR (S):

SOURCE:

methallyl dichloride Surapaneri, Rao; Damavarapu, Reddy; Duddu, Raja; Dave,

Paritosh R.; Gilardi, Richard D.

CORPORATE SOURCE:

WS Army Armament Research Development and Engineering

Center, Picatinny Arsenal, NJ, 07806-5000, USA International Annual Conference of ICT (2002)

33rd(Energetic Materials), 147/1-147/5

CODEN: IACIEQ; ISSN: 0722-4087

PUBLISHER:

Fraunhofer-Institut fuer Chemische Technologie

Journal DOCUMENT TYPE: LANGUAGE: English

Several polynitrato and polyazido compds., derived from a lower homolog of pentaerythritol and have one less methylene unit, were synthesized in order to develop lead-free primary explosives. The compds. were derived from methallyl dichloride by such reactions as epoxidn., nucleophilic substitution, and ring-opening nitration. Nitration. These compds. are of potential interest as energetic plasticizers and their multiple functional groups can be exploited to prepare novel dendritic structures.

L19 ANSWER 8 OF 20 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2001:99711 HCAPLUS

DOCUMENT NUMBER: 134:297035

TITLE: Azido-containing polyurethanes

AUTHOR(S): Tselinskii, I. V.; Bestuzheva, V. V.; Nalimova, N. K.;

Skirdova, G. V.

CORPORATE SOURCE: St. Peterburg. Gos. Tekhnol. Inst., Russia

SOURCE: Zhurnal Prikladnoi Khimii (Sankt-Peterburg, Russian

Federation) (2000), 73(12), 2057-2060

CODEN: ZPKHAB; ISSN: 0044-4618

PUBLISHER: Nauka
DOCUMENT TYPE: Journal
LANGUAGE: Russian

AB High energy polyurethane elastomers with good mech. strength were prepared by reacting poly(butylene ethylene adipate) with a diisocyanate (HMDI, MDI, TDI) and a crosslinker (glycerol, pentaerythritol) in the presence of azide plasticizers. The polymers can be used as binders for rocket fuel.

L19 ANSWER 9 OF 20 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1995:830797 HCAPLUS

DOCUMENT NUMBER: 123:291159

TITLE: Development of energetic additives for propellants in

China

AUTHOR(S): Ou, Yuxiang; Chen, Boren; Yan, Hong; Jia, Huiping; Li,

Jianjun; Dong, Shuan

CORPORATE SOURCE: Department Chemical Engineering, Beijing Institute

Technology, Beijing, 100081, Peop. Rep. China

SOURCE: Journal of Propulsion and Power (1995), 11(4), 838-47

CODEN: JPPOEL; ISSN: 0748-4658

PUBLISHER: American Institute of Aeronautics and Astronautics

DOCUMENT TYPE: Journal LANGUAGE: English

AB The development of energetic azide binders and plasticizers for solid propellants in China was described, focusing on 14 azides. The reaction routes and conditions for preparing these azides were summarized; the performance of the azides, including d., m.p., enthalpy of formation, thermal decomposition temperature (determined by differential scanning calorimetry or

DTA), impact sensitivity, etc, were presented. The azides were arranged in six categories: (1) azide polyethers (glycidyl azide polymer, 3,3-bis(azidomethyl)oxetane (BAMO) homopolymer, and BAMO-tetrahydrofuran copolymer), (2) azidonitramines (1,5-diazido-3-nitrazapentane, N-nitro-N-azidomethyl-gem-dinitroethylmethylamine, and N,N'-bis(azidomethyl-gem-dinitroethyl)ethylenedinitramine), (3) azidonitro compds. [2-nitro-2-methyl-1,3-diazidopropane, 2-nitro-2-azidomethyl-1,3-diazidopropane, and 1-azido-2-(2,4,6-trinitrophenyl)ethane], (4) aliphatic azides (1,2,4,triazidobutane and tetraazidomethylemethane), (5) azidonitrates (pentaerythritol diazidodinitrate), and (6) oxygen heterocyclic azides (3-azidomethyl-3-ethyloxetane and 2,2-dimethyl-5-azidomethyl-5-nitro-1,3-dioxane).

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L19 ANSWER 10 OF 20 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1995:767546 HCAPLUS

DOCUMENT NUMBER: 123:183322

TITLE: Photographic processing compositions and processing

method

INVENTOR(S): Inaba, Tadashi

PATENT ASSIGNEE(S): Fuji Photo Film Co Ltd, Japan SOURCE: Jpn. Kokai Tokkyo Koho, 41 pp.

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11/17/2005

10604774.trn

CODEN: JKXXAF

DOCUMENT TYPE:

Patent

Japanese

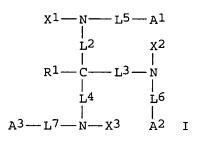
LANGUAGE:

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 07114162	A2	19950502	JP 1993-262688	19931020
PRIORITY APPLN. INFO.:			JP 1993-262688	19931020
OTHER SOURCE(S):	MARPAT	123:183322		

GI



· AB The title compns. contain at least one kind of I [R1 = H, substituent; X1-3 = H, L1A; L1-7 = divalent aliphatic, divalent aromatic; A, A1-3 = CO2H, OM,

SO3M, PO(OM)2; M = H, cation] or its chelate compound with Fe(III), Mn(III), Co(III), Rh(II), Au(II), or Ce(IV). A bleaching agent may contain the above compns.

L19 ANSWER 11 OF 20 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

1995:705389 HCAPLUS

DOCUMENT NUMBER:

123:97788

TITLE:

Photographic processing material

INVENTOR(S):

Inaba, Tadashi

PATENT ASSIGNEE(S): SOURCE:

Fuji Photo Film Co Ltd, Japan Jpn. Kokai Tokkyo Koho, 33 pp.

CODEN: JKXXAF

DOCUMENT TYPE:

Patent

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	. DATE	
JP 07114154	A2	19950502	JP 1993-259956	19931018	
PRIORITY APPLN. INFO.:			JP 1993-259956	19931018	
GI					

AB The title processing material contains a compound I (R1 = H, substitute; X1-3 = H, -L1-A; L1-7 = divalent group; A, A1-3 = CO2M, OM, SO3M, PO(OM)2; M = cation) or its salt. The invention processing material can prevent mold and bacteria generation and photog. characteristics deterioration caused by metal ions.

L19 ANSWER 12 OF 20 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1994:523819 HCAPLUS

DOCUMENT NUMBER: 121:123819

TITLE: Macrobicyclic cobalt(III) hexaamine complexes based on

tris(propylenediamine)cobalt(III)

AUTHOR(S): Benjarvongkulchai, Soontaree; Kaewhom, Anusak;

Waitayasuwan, Patranit

CORPORATE SOURCE: Fac. Sci., Silpakorn Univ., Nakorn Pathom, 73000,

Thailand

Journal

SOURCE: Journal of the Science Society of Thailand (1992),

18(3), 151-61

CODEN: VKSTDB; ISSN: 0303-8122

DOCUMENT TYPE:

LANGUAGE: English

AB The cage complexes: Δ , fac-lel3-[Co(NO2)2Me3sar]3+ (1) ((NO2)2Me3sar

= 1,8-dinitro-(4R,12R,17R)-trimethyl-3,6,10,13,16,19-

hexaazabicyclo[6.6.6]eicosane) and Δ , fac-lel3-[Co(Me3sep)]3+ (3)

(Me3sep = (4R, 12R, 17R) - trimethyl - 1, 3, 6, 8, 10, 13, 16, 19 -

octaazabicyclo[6.6.6]eicosane) and their corresponding halfcage complexes:

 Δ , fac-lel3-[Co(NO2Me3semisar)]3+ (2) (NO2Me3semisar =

tris(((2-aminopropyl)amino)methyl)nitromethane) and Δ , fac-lel3-

[Co(Me3semisep)]3+(4) (Me3semisep = tris(((2-

aminopropyl)amino)methyl)amine) are synthesized from Δ , fac-lel3-[Co(R)(-)pn3]3+. Likewise their Λ -enantiomers are synthesized from Λ , fac-lel3[Co(S)(+)pn3]3+. The sp. rotations, IR spectra, visible

spectra, NMR spectra and oxidation-reduction potentials are recorded.

L19 ANSWER 13 OF 20 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1994:181567 HCAPLUS

DOCUMENT NUMBER: 120:181567

TITLE: Structural characterization of encapsulation reactions

based on the tris(ethane-1,2-diamine)cobalt(III) ion Clark, Ian J.; Geue, Rodney J.; Engelhardt, Lutz M.; Harrowfield, Jack M.; Sargeson, Alan M.; White, Allan

Η.

CORPORATE SOURCE: Dep. Chem., Univ. West. Australia, Nedlands, 6009,

Australia

SOURCE: Australian Journal of Chemistry (1993), 46(10),

1485-505

CODEN: AJCHAS; ISSN: 0004-9425

AUTHOR (S):

DOCUMENT TYPE:

Journal

LANGUAGE:

English

GI

AB From structural comparisons involving intermediates and side products of encapsulation (clathrochelation) reactions as well as several cage complexes, the efficiency of the base-catalyzed reaction between formaldehyde, nitromethane and [Co(en)3]3+ to give [Co((NO2)2sar)]3+ [(NO2)2sar = I, X = CNO2] appears to be explicable in terms of the 'interlocking' of constituent parts without appreciable concomitant bond length or bond angle distortions. Crystal structures were determined for Λ -[Co(NO2sen)]Cl3·2H2O [NO2sen = O2NC(CH2NHCH2CH2NH2)3] and Δ, Λ -[CoL]Cl3.nH2O (L = I; X = CNO2, n = 2; X = OH, n = 3), and Δ, Λ -[CoL'] (NO3)3 (L' = II) and 2 related complexes. The structures show very close configurational and conformational similarities to each other as well as to published structures of [Co(en)3]3+, [Co(tame)2]3+ (tame = 1,1,1-tris(aminomethyl)ethane) and other cage complexes. Some of these similarities may be associated with common hydrogen-bonding patterns in the solids resulting from anion 'chelation' by adjacent NH moieties in the metal ion coordination spheres. Necessary caution in relating structural and electronic properties is implied by the structure determination for Δ, Λ -[CoL'] (NO3)3 [monoclinic, P21/c, R = 0.061], one of the products of mol. rearrangement following nitrosation of [Co((NH2)2sar)]3+. Despite marked electronic spectral and electrochem. differences with its parent complex, [CoL'] (NO3)3 contains cobalt(III) in a coordination environment which remains similar to those in more sym. cage complexes.

L19 ANSWER 14 OF 20 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

1991:217995 HCAPLUS

DOCUMENT NUMBER:

114:217995

TITLE:

Silver halide photographic materials containing

rapid-acting vinyl sulfone hardening agent

Nishizeki, Masahito; Tachibana, Noriki; Kagawa,

Nobuaki

PATENT ASSIGNEE(S):

Konica Co., Japan

SOURCE:

Jpn. Kokai Tokkyo Koho, 18 pp.

CODEN: JKXXAF

DOCUMENT TYPE:

INVENTOR(S):

Patent

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE JP 02238451 ---------A2 19900920 JP 1989-57891 19890313 PRIORITY APPLN. INFO.: JP 1989-57891 19890313

MARPAT 114:217995 OTHER SOURCE(S):

The photog. material has ≥1 component layer(s) hardened with CH2: CHSO2CH2CONRCH2CR1 (OH) [ZCR2 (OH)] mCH2NR3COCH2SO2CH: CH2 and/or CH2: CHSO2CH2CONR4CH (CH2OH) [Z1CH (CH2OH)] nNR5COCH2SO2CH: CH2 (R, R3-5 = H, R3-5 = H, R3-5 = R, R3-5 =C1-4 hydrocarbon, CH2:CHSO2CH2CO; R + R3, R4 + R5 may be C1-4 alkylene and form rings; R1, R2 = H, C1-4 alkyl, CH2:CHSO2CH2CONR6CH2; R6 = H, C1-4 hydrocarbon; Z, Z1 = organic moiety, bivalent linkage group; m, n = 0, 1).

L19 ANSWER 15 OF 20 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1990:601276 HCAPLUS

DOCUMENT NUMBER: 113:201276

TITLE:

Silver halide photographic materials containing

water-soluble vinyl sulfone hardeners

INVENTOR(S):

Nishizeki, Masahito; Tachibana, Noriki; Kagawa,

Nobuaki

PATENT ASSIGNEE(S):

Konica Co., Japan

SOURCE:

Jpn. Kokai Tokkyo Koho, 18 pp.

CODEN: JKXXAF

DOCUMENT TYPE:

Patent Japanese

LANGUAGE:

FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION:

KIND DATE APPLICATION NO. DATE PATENT NO. ---------------JP 02110545 PRIORITY APPLN. INFO.: 19900423 JP 1988-262821 19881020 JP 1988-262821 19881020 A2

The title materials comprise supports and ≥1 layer hardened with vinyl sulfones of the formula (CH2:CHSO2CH2CONR)nZ (I; R = H, C1-4 hydrocarbon residue, CH2:CHSO2CH2CH2CO; Z = a di- to tetravalent OH-substituted organic group; n = 2, 3, 4). Thus, high-speed color neg. films, prepared by addition of the vinyl sulfone I [R = H; Z = CH2CH(OH)CH2; n = 2] to each component layer, showed excellent antifogging characteristics and high strength.

L19 ANSWER 16 OF 20 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1989:174257 HCAPLUS

DOCUMENT NUMBER:

110:174257

TITLE:

Synthesis of the macroporous polystyrene strongly basic anion exchanger (type 1) with high exchange

capacity

AUTHOR(S):

Jin, Qunying; Tang, Guoan

CORPORATE SOURCE:

Inst. Sci., Yibin Tianyuan Chem. Plant, Peop. Rep.

China

SOURCE:

Lizi Jiaohuan Yu Xifu (1987), 3(2), 9-13

CODEN: LJYXE5; ISSN: 1001-5493

DOCUMENT TYPE:

Journal

LANGUAGE: Chinese

AB The title anion exchanger was prepared by suspension polymerization of styrene with

divinylbenzene followed by chloromethylation and amination of the resultant copolymer. The anion exchanger had an ion-exchange capacity 4-4.4 meg/g resin, surface area 40-50 m2/g, and average pore radius 90-100 A. The chemical and phys. properties of the anion exchanger were similar

with those of Amberlite IRA 900C resin. Paraffin and petroleum liqs. were used as pore-forming agents.

L19 ANSWER 17 OF 20 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1976:67790 HCAPLUS

DOCUMENT NUMBER: 84:67790

TITLE: Diffusion transfer color film unit

INVENTOR(S):
Ono, Yoshiaki

PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan

SOURCE: Ger. Offen., 92 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2455022	A1	19750522	DE 1974-2455022	19741120
JP 50081537	A2	19750702	JP 1973-130379	19731120
US 3960569	Α	19760601	US 1974-525431	19741120
GB 1480370	Α	19770720	GB 1974-50378	19741120
PRIORITY APPLN. INFO.:			JP 1973-130379	A 19731120

The fast formation of diffusion-transfer color images having high contrast AB is achieved by using a phys. developer containing an alkanolamine as developer accelerator at 0.05-3 g/l. of processing solution Especially useful as the accelerator is N-(aminoethyl)ethanolamine. Thus, a color diffusion-transfer film unit, which was described in detail, was imagewise exposed and then developed by rupturing a pod contg.a processing solution of the following composition: ascorbic acid 20, 6-nitrobenzimidazole nitrate 15 mg, Na2S2O3 0.8, TiO2 3, NaOH 4, CM-cellulose Na salt 3.5, 4-amino-3-methyl-N-ethyl-N-(β -hydroxyethyl)aniline sulfate 3 g, N-(aminotheyl)ethanolamine 0.1 ml, and water 100 ml. The red, green, and blue Dmax values were 1.60, 1.65, and 1.60, resp.; the red, green, and blue Dmin values were 0.15, 0.17, and 0.22, resp.; and the red, green, and blue contrast values 1.45, 1.48, and 1.38 vs. 1.40, 1.40, and 1.30, resp.; 0.20, 0.40, and 0.35, resp.; and 1.20, 1.00, and 0.95, resp., for an N-(aminoethyl)ethanolamine-free control.

L19 ANSWER 18 OF 20 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1972:513928 HCAPLUS

DOCUMENT NUMBER: 77:113928

TITLE: Synthesis of quaternary ammonium compounds containing

a nitrodiaminopropane component Torf, S. F.; Cherepanova, V. P.

AUTHOR(S): Torf, S. F.; Cherepanova, V. P. CORPORATE SOURCE: Inst. Eksp. Med., Leningrad, USSR

SOURCE: Khimiko-Farmatsevticheskii Zhurnal (1972), 6(7), 27-9

CODEN: KHFZAN; ISSN: 0023-1134

DOCUMENT TYPE: Journal LANGUAGE: Russian

AB Reaction of (HOCH2)2C(Me)NO2 (I) with p-(Me2N)2C6H4 (II) and p-(Et2N)2C6H4 and of (HOCH2)3CNO2 with II gave (RC6H4NHCH2)2C(Me)NO2 (III, R = Me2N, Et2N) and (RC6H4NHCH2)3CNO2 (IV, R = Me2N), resp., MeI derivs. of which at 1.0, 0.7, and 0.3 mg/kg had curare-form activity equal to (IV, less toxicity than) 0.1 mg d-tubocurarine/kg.

L19 ANSWER 19 OF 20 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1959:4350 HCAPLUS

DOCUMENT NUMBER: 53:4350

ORIGINAL REFERENCE NO.: 53:770i,771a-b

TITLE: Polyepoxide-treated amine-modified thermoplastic

phenol-aldehyde resins

INVENTOR (S): De Groote, Melvin; Shen, Kwan-Ting

PATENT ASSIGNEE(S): Petrolite Corp.

DOCUMENT TYPE: Patent LANGUAGE: Unavailable

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

KIND PATENT NO. DATE APPLICATION NO. DATE ----------

US 2828276 19580325 US

GI For diagram(s), see printed CA Issue.

AB Cf. U.S. 2,771,437 (C.A. 51, 4690b). Phenol-aldehyde, resins were condensed with basic nonhydroxylated secondary polyamines and HCHO, followed by reaction with phenolic diepoxides to give products useful for breaking petroleum emulsions or as detergents, emulsifying, or wetting agents. A phenol-aldehyde resin (882 g.) (from p-Me3CC6H4OH and HCHO), 600 xylene, 176 (MeNHCH2)2, and 200 g. of 30% HCHO were heated for 19 h. at 80-46° and refluxed with removal of water. The condensate 116 g. in xylene was treated at 100-60° with 17 g. (p-O.CH2.CHCH2OC6H4)2CMe2 (I) for 6 h. to give a product represented by [(Amine) CH2 (Resin) CH2 (Amine)]2 DGE, where DGE is diglycidyl ether, a dark-red, viscous semisolid, insol. in H2O, soluble in xylene: MeOH 8:2 plus 5% gluconic acid. U.S. 2,828,277 relates to use of hydroxylated polyamines, such as (HOC2H4NHCH2)2; U.S. 2,828,280 to amines, such as NH(C2H4OH)2; U.S. 2,828,281 to amines, such as Et2NH; and U.S. 2,828,282 to cyclic amidines. U.S. 2,828,283 relates to products from I and phenol-aldehyde resins and their hydroxyalkylation derivs., without amine modification.

L19 ANSWER 20 OF 20 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1949:15059 HCAPLUS

DOCUMENT NUMBER: 43:15059

ORIGINAL REFERENCE NO.: 43:2935h-i,2936a-f

TITLE: Derivatives of tris(hydroxymethyl)nitromethane

AUTHOR (S): Fort, Godfrey; McLean, Andrew

SOURCE: Journal of the Chemical Society, Abstracts (1948)

1902-7

CODEN: JCSAAZ; ISSN: 0590-9791

DOCUMENT TYPE: Journal LANGUAGE: Unavailable GT

For diagram(s), see printed CA Issue. AB

(HOCH2)3CNO2 (I) and SOC12 in C5H5N, kept overnight at 40-50° and 1 hr. at 95-100°, give 72.5% (C1CH2)3CNO2 (II), m. $102-4\degree$; a by-product (sometimes the main product) is 2-nitro-2-(chloromethyl)trimethylene sulfate, SO2(O.CH2)2C(NO2)CH2Cl, m. 86-9°. I (0.95 mol.), 2 mols. SOCl2, and 2.1 mols. C5H5N give 28% 2-nitro-2-(hydroxymethyl)trimethylene sulfate, m. 105-6°. Fe (100 g.) activated with concentrated HCl, added to 25 g. II in 400 cc. C6H6 and the mixture treated with 40 cc. H2O (2 cc. at 15-min. intervals), gives 82.5% (ClCH2)3CNH2 (III), pale yellow, b6.5 75-84°; SnCl2 in EtOH gives 65% III. Equivalent quantities of III and m-O2NC6H4CHO in EtOH, refluxed 2.5 hrs., give 70.5% N-(m-nitrobenzylidene)tris(chloromethyl)aminomethane, m. 83-4.5°. III (5 g.), heated 7 hrs. at 120°, gives 12% 2,2,5,5-tetrakis(chloromethyl)piperazine (IV), m. 105-6°, and 1.06 g. of the HCl salt of III; other methods for the preparation of IV are given. IV and BzCl in C5H5N give a compound m. 210-15° (decomposition);

p-MeC6H4SO2Cl in C5H5N gives the monotosyl derivative, m. 138-40°, and the ditosyl derivative, m. 250° (decomposition). III and p-MeC6H4SO2Cl in C5H5N, kept 2 days, give 94% tris(chloromethyl)-p-tolylsulfonamidomethane (V), m. 134-5°. V and p-MeC6H4SO2NHNa, heated 10 hrs. at 140°, give 64% tris(p-tolylsulfonamidomethyl)-ptolylsulfonamidomethane (VI), m. 197-8°; at 170 and 210° the yields are 38 and 24%, resp.; in boiling EtOH containing excess NaOH (9 hrs.) the yield is 42.4%. V and p-MeC6H4SO2NMeNa (10 hrs. at 140°) give 14% tris(N-methyl-p-tolylsulfonamidomethyl)-p-tolylsulfonamidomethane, m. 195°. VI (8 g.) and 24 cc. 80% H2SO4, heated 3 hrs. at 200°, give 85.5% of the disulfate (VII), m. 280° (decomposition), of tris(aminomethyl)aminomethane (VIII), b3-4 120°. III (4 g.) in 23 cc. EtOH and 70 cc. NH4OH (d. 0.88), heated 3 hrs. at $100-10^{\circ}$ and the residue treated with ${\tt H2SO4}$, give 91% VII. With excess ${\tt Ba}({\tt OH})\,{\tt 2}$ in hot H2O, VII gives 95% VIII; KOH gives 73%; VIII is best prepared from III without isolation of VII; tetrapicrate of VIII m. 140° tetra-HCl salt m. 270° (decomposition). The high-boiling fraction from VIII and p-MeC6H4SO2Cl gives the hexatosyl derivative, C50H61O12N7S6, m. 275-8°, of the secondary amine, [(H2NCH2)3C]2NH, derived from VIII by elimination of NH3. VIII (4.85 g.) in 80 cc. H2O containing 6.6 g. NaOH, treated (0.5 hr.) at 0-10° with 15.6 cc. ClCO2Et (100 cc. ether added midway during the reaction) and the mixture stirred 2 hrs., gives 52% tris(carbethoxyaminomethyl)carbethoxyaminomethane (IX), m. 145-6°; simultaneous addition of HCO2Et and alkali gives 20% IX and 1,3-bis[tris(carbethoxyaminomethyl)methyl]urea, m. 272° (decomposition). IX, added to HNO3 and Ac2O at 0 $^{\circ}$, gives a sticky gum; (O2NNHCH2)3CNHNO2 was not formed. (HOCH2)3CNH2 and HCHO give 7a-(hydroxymethyl)-2,6-dioxapyrrolizidine (X); methiodide m. 215° (decomposition); acetate m. 94-5°. X (4 g.), added to 30 cc. HNO3 (d. 1.52) and 25 cc. concentrated H2SO4 at 0-5° (15-30 min.), give 22% 3-nitro-4,4-bis(nitroxymethyl)oxazolidine, O2NN.CH2.O.CH2.C(CH2ONO2)2, m. 67.5-70°.

```
=> s polyazido
```

L21 18 POLYAZIDO

=> s 121 and azide

40607 AZIDE

8478 AZIDES

42978 AZIDE

(AZIDE OR AZIDES)

L22 9 L21 AND AZIDE

=> s 121 and py<=2002

22790379 PY<=2002

L23 11 L21 AND PY<=2002

=> d 121 ibib abs hitstr tot

L21 ANSWER 1 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2005:921122 HCAPLUS

TITLE: Synthesis, Characterization, and Energetic Properties

of Diazido Heteroaromatic High-Nitrogen C-N Compound Huynh, My Hang V.; Hiskey, Michael A.; Chavez, David

AUTHOR(S): Huynh, My Hang V.; Hiskey, Michael A.; C E.; Naud, Darren L.; Gilardi, Richard D.

CORPORATE SOURCE: Dynamic Experimentation Division DX-2: Materials

Dynamics, Los Alamos National Laboratory, Los Alamos,

NM, 87545, USA

SOURCE: Journal of the American Chemical Society (2005)

127(36), 12537-12543

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal LANGUAGE: English

The synthesis, characterization, and energetic properties of diazido heteroarom. high-nitrogen C-N compound, 3,6-diazido-1,2,4,5-tetrazine

(DiAT), are reported. Its normalized heat of formation (N Δ Hf),

exptl. determined using an additive method, is shown to be the highest pos.

NAHf compared to all other organic mols. The unexpected

azido-tetrazolo tautomerizations and irreversible tetrazolo transformation of DiAT are remarkable compared to all other polyazido

heteroarom. high-nitrogen C-N compds., for example, 2,4,6-triazido-1,3,5triazine; 4,4',6,6'-tetra(azido)hydrazo-1,3,5-triazine;

4,4',6,6'-tetra(azido)azo-1,3,5-triazine; and 2,5,8-tri(azido)-

1,3,4,6,7,9,9b-heptaazaphenalene.

REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 2 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

2005:101974 HCAPLUS

DOCUMENT NUMBER:

142:359349

TITLE:

Preparation of nitrogen-rich nanolayered,

nanoclustered, and nanodendritic carbon nitrides

AUTHOR (S):

Huynh, My Hang V.; Hiskey, Michael A.; Archuleta, Jose

G.; Roemer, Edward L.

CORPORATE SOURCE:

Dynamic Experimental Division, DX-2: Materials

Dynamics Group, Los Alamos National Laboratory, Los

Alamos, NM, 87545, USA

SOURCE:

Angewandte Chemie, International Edition (2005),

44(5), 737-739

CODEN: ACIEF5; ISSN: 1433-7851 Wiley-VCH Verlag GmbH & Co. KGaA

PUBLISHER: DOCUMENT TYPE:

Journal

LANGUAGE: English

AB Only C and N atoms are present in the high-nitrogen compound 4,4',6,6'-tetra(azido)azo-1,3,5-triazine (TAAT), which is thus an ideal precursor for carbon nitrides. Controlled pyrolysis of TAAT afforded novel nitrogen-rich carbon nitrides in the form of nanolayers (C2N3), nanoclusters (C3N5), and nanodendrites (C3N5). The pyrolyzes occur at low temperature and without applied pressure and require no vacuum systems,

extraction,

carbonization, or purification

REFERENCE COUNT:

26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 3 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

2005:29032 HCAPLUS

DOCUMENT NUMBER:

142:114074

TITLE:

Preparation of polyazido carboxylic acid

esters Dave, Paritosh R.; Duddu, Raja G.; Damavarapu, Reddy;

Gelber Nathaniel; Yang, Kathy; Surapaneni, C. Rao

United States Dept. of the Army, USA

PATENT ASSIGNEE(S):

SOURCE:

Ü.S., 9 pp. CODEN: USXXAM

DOCUMENT TYPE:

INVENTOR(S):

Patent

LANGUAGE:

English

10604774.trn

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10:44

FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION:



Y X
$$\frac{Z}{N}$$
 $\frac{DH}{N}$ $\frac{DH}{$

AB This invention relates to a series of novel compds., such as I = X = XOH, ONO2, NO2; Y = CH2N3, NO2; A, B = N3, 4-carboxytriazolomethyl], and II [Z = CH2, O, NOH, 2,4-dihydrophenylhydrozono], including 2-azido-2-azidomethyl-1,3-diazidopropane, 2-azidomethyl-2-hydroxy-1,3diazidopropane, 2-azidomethyl-2-nitrato-1,3-diazidopropane, 2-azidomethyl-2-nitro-1,3-diazidopropane, 2,2-dinitro-1,3-diazidopropane, methallyidiazide, a dimer of methallyidiazide, comprising 3a,8a-bis-azidomethyl-3a,4,8a,9-tetrahydro-3H,8H-bis[1,2,3]triazolo[1,5-a; 1'',5''-d]pyrazine, 1,3-diazidoacetone, and 2-oximido-1,3-diazidopropane. Also shown are reaction intermediates of these compds., including 2,2-bis(chloromethyl)oxirane, and 2,2-bis(azidomethyl)oxirane. In addition, a number of potentially useful energetic compds. have been prepared from the low mol. weight polyazido compds. above, including N-2(azido-1-azidomethyl-ethylidene)-N''-(2,4-dinitrophenyl)-hydrazine (7-DNPH), 1,3-bis(4-carboxytriazolyl)2,2-dinitropropane, tris(4-carboxytriazolomethyl)methanol, benzene-1,3,5-tricarboxylic acid tris(2-azido-1,1-bisazidomethyl-ethyl)ester, adamantane 1,3,5,7-tetracarboxylic acid tetrakis(2-azido-1,1-bisazidomethylethyl)ester, adamantane carboxylic acid (2-azido-1,1-bisazidomethylethyl)ester, cubane 1,3,5,7-tetracarboxylic acid tetrakis (2-azido-1,1-bisazidomethyl-ethyl)ester, cubane 1,4-dicarboxylic acid bis(2-azido-1,1-bisazidomethyl-ethyl)ester. Thus, tris(4carboxytriazolomethyl) methanol (III) was prepared by the reaction of 2-azidomethyl-2-hydroxy-1,3-diazidopropane I [A, B = N3; X = CH2N3; Y = OH] (also prepared) with propiolic acid. REFERENCE COUNT: THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS

L21 ANSWER 4 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:809497 HCAPLUS

DOCUMENT NUMBER: 141:334417

TITLE: Polyazido high-nitrogen compounds: hydrazo-

and azo-1,3,5-triazine

AUTHOR(S): Huynh, My-Hang V.; Hiskey, Michael A.; Hartline,

Ernest L.; Montoya, Dennis P.; Gilardi, Richard

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

CORPORATE SOURCE: Dynamic Experiment Division, Los Alamos National

10604774.trn

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10:44

Laboratory, Los Alamos, NM, 87545, USA

SOURCE: Angewandte Chemie, International Edition (2004),

43(37), 4924-4928

CODEN: ACIEF5; ISSN: 1433-7851 PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:334417

The synthesis and properties of novel 4,4',6,6'-tetra(azido)hydrazo-1,3,5triazine and 4,4',6,6'-tetra(azido)azo-1,3,5-triazine (I), both with 6 carbon atoms and 20 nitrogen atoms, were reported, from hydrazinolysis of 4,4',6,6'-tetrachlorohydrazo-1,3,5-triazine. The two products demonstrated that hydrazo and azo linkages can be used to desensitize

polyazido high-nitrogen compds., and also decrease their

volatility. I had the highest exptl. measured heat of formation reported

for energetic organic compds. (+2171 kJ/mol).

REFERENCE COUNT: THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS 37 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 5 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:809494 HCAPLUS

DOCUMENT NUMBER: 141:381721

TITLE: High-energy-density materials: synthesis and

characterization of N5+[P(N3)6]-, N5+[B(N3)4]-,

N5+[HF2]-nHF, N5+[BF4]-, N5+[PF6]-, and

N5 + [SO3F] -

AUTHOR (S): Haiges, Ralf; Schneider, Stefan; Schroer, Thorsten;

Christe, Karl O.

Loker Research Institute, University of Southern CORPORATE SOURCE:

California, Los Angeles, CA, 90089-1661, USA Angewandte Chemie, International Edition (2004),

43(37), 4919-4924

CODEN: ACIEF5; ISSN: 1433-7851 Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal LANGUAGE: English

SOURCE:

PUBLISHER:

A number of pentanitrogen cation, N5+, with energetic polyazido anions, [P(N3)6] - and [B(N3)4] -, as well as other N5+ salts with [HF2] - .nHF, [BF4] -, [PF6] -, and [SO3F] -. The [P(N3)6] - and [B(N3)4] -

salts contained 91 and 96 weight% N, resp. The thermally unstable compound N5+HF2.nHF was prepared by metathesis from N5SbF6 and CsHF2. Its usefulness

as a reagent for the synthesis of new N5+ salts was demonstrated.

REFERENCE COUNT: 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 6 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:137939 HCAPLUS

DOCUMENT NUMBER: 140:357709

TITLE: Preparation of cage molecule based polyazido

core units for dendrimer synthesis

AUTHOR (S): Dave, Paritosh R.; Duddu, Raja; Yang, Kathy;

Damavarapu, Reddy; Gelber, Nathaniel; Surapaneni, Rao;

Gilardi, Richard

CORPORATE SOURCE: GEO-CENTERS, INC. at ARDEC, Picatinny Arsenal, NJ,

07806-5000, USA

SOURCE: Tetrahedron Letters (2004), 45(10), 2159-2162

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

Core mols. based on benzene-, cubane-, and adamantane-polycarboxylates with peripheral polyazido substitution were prepared The first synthesis of 1,3-diazidoacetone and its conversion to the corresponding oxime, DNPH, and 2,2-dinitro derivs. is also reported. All azido compds. should be considered dangerous and proper precautions should be taken during handling and storage of these mols.

REFERENCE COUNT:

17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 7 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

2003:183497 HCAPLUS

TITLE:

Main-group polyazido compounds

AUTHOR (S):

Haiges, Ralf; Boatz, Jerry A.; Christe, Karl; Gerken,

M.; Schneider, Stefan; Schroer, Thorsten; Tham, Fook

S.; Vij, Ashwani

CORPORATE SOURCE:

Loker Hydrocarbon Research Institute, University of Southern California, Los Angeles, CA, 90089, USA

SOURCE:

Abstracts of Papers, 225th ACS National Meeting, New Orleans, LA, United States, March 23-27, 2003 (2003)

INOR-454. American Chemical Society: Washington, D.

CODEN: 69DSA4

DOCUMENT TYPE:

Conference; Meeting Abstract

LANGUAGE:

English

AB The preparation of main group polyazido compds. will be reported. Their phys., spectroscopic and structural properties as well as theor. calcns. will be discussed.

L21 ANSWER 8 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

2002:605702 HCAPLUS

DOCUMENT NUMBER:

138:75615

TITLE:

Novel polyazido/polynitrato compounds

derived from methallyl dichloride

AUTHOR (S):

Surapaneni, Rao; Damavarapu, Reddy; Duddu, Raja; Dave

Paritosh R Gilardi, Richard D.

CORPORATE SOURCE:

US Army Armament Research Development and Engineering Genter, Picatinny Arsenal, NJ, 07806-5000, USA

International Annual Conference of ICT (2002),

33rd(Energetic Materials), 147/1-147/5 CODEN: IACIEQ; ISSN: 0722-4087

PUBLISHER:

SOURCE:

Fraunhofer-Institut fuer Chemische Technologie

DOCUMENT TYPE:

Journal

LANGUAGE:

English

AB Several polynitrato and polyazido compds., derived from a lower homolog of pentaerythritol and have one less methylene unit, were synthesized in order to develop lead-free primary explosives. The compds. were derived from methallyl dichloride by such reactions as epoxidn., nucleophilic substitution, and ring-opening nitration. Nitration. These compds. are of potential interest as energetic plasticizers and their multiple functional groups can be exploited to prepare novel dendritic structures.

L21 ANSWER 9 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

1997:102122 HCAPLUS

DOCUMENT NUMBER:

126:188091

TITLE:

High-energy hydroxy-terminated polyazido polymers used as binder for propellants

INVENTOR (S):

Huang, Der-shing; Rindone, Renato R.

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PATENT ASSIGNEE(S): Aerojet-General Corporation, USA

SOURCE: U.S., 10 pp., Cont.-in-part of U.S. Ser. No. 686,953,

abandoned.

CODEN: USXXAM

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. --------------US 5597978 Α 19970128 US 1987-98529 19870918 PRIORITY APPLN. INFO.: US 1984-686953 B2 19841227

 $\label{thm:hydroxy-terminated} \mbox{ aliphatic polyethers have the formula HO(CR1R4CR2R4O)} \ n\mbox{H}$ AB where R1, R2, R3, and R4 are independently selected from H, CH2N3, and CHN3CH2N3, the total number of azide groups per monomer unit is 2-3, and n is an integer 2-40. Copolymers of the monomer units in the above formula with other, known azido-substituted monomer units further provide energy outputs at preselected levels based on the proportions of each type of monomer present.

L21 ANSWER 10 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1996:285147 HCAPLUS

DOCUMENT NUMBER: 124:320922

TITLE: Synthesis of homocubane-based energetic molecules AUTHOR (S): Guan, Xiaopei; Du, Jianwei; Sun, Jianguang: Su.

Zhuang; Yu, Yongzhong

CORPORATE SOURCE: Beijing Institute Technology, College Chemical

Engineering and Materials Science, Beijing, 100081,

Peop. Rep. China

SOURCE: Proceedings of the Beijing International Symposium on

Pyrotechnics and Explosives, 3rd, Beijing, Nov. 6-9, 1995 (1995), 139-142. Editor(s): Yuxiang, Ou. China

Ordnance Society: Beijing, Peop. Rep. China.

CODEN: 62RIAT

DOCUMENT TYPE: Conference LANGUAGE: English

Energetic homocubane derivs. were synthesized and characterized for use as explosives and propellant ingredients. Six polynitro and polyazido diesters of homocubane-2,4-dicarboxylic acid were synthesized as possible energetic plasticizers; 2,4-dicyano and dinitro homocubanes were also synthesized as models for more highly substituted homocubanes. Dinitrate and diperchlorate salts of 2,4-diaminohomocubane were prepared via ion exchange. Further nitration of 2,4bis(fluorodinitroethylamino)homocubane and homocubane-2,4-bis(Ntrinitroethylamide) is in progress.

L21 ANSWER 11 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1996:215534 HCAPLUS

DOCUMENT NUMBER: 125:11288

TITLE: Chemoenzymic methods for the preparation of optically

active cyclic polyazido alcohols from easily

available achiral starting materials

AUTHOR (S): Gruber-Khadjawi, Mandana; Honig, Helmut; Illaszewicz,

Carina

CORPORATE SOURCE: Inst. Org. Chem., Tech. Univ. Graz, Graz, A-8010,

Austria

SOURCE: Tetrahedron: Asymmetry (1996), 7(3), 807-14

CODEN: TASYE3; ISSN: 0957-4166

10604774.trn Page 68 10:44

PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Optically active 2,5-diazido-1,4-cyclohexanediol, 4,6-diazido-1,3-cyclohexanediol and 2,5-diazido-1,4-cyclohexanediol as precursors for polyfunctional cyclic amino alcs. were prepared by enzymic hydrolysis of the resp. butyrates with lipases from Candida rugosa (CRL), Pseudomonas cepacia (PCL), and Geotrichum candidum (GCL). The enantiomeric excesses obtained were very high.

L21 ANSWER 12 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1995:371347 HCAPLUS

DOCUMENT NUMBER: 122:213678

TITLE: Studies on reactions of polynitrostilbenes with sodium

azide

AUTHOR(S): Zengguo, Feng; Boren, Chen

CORPORATE SOURCE: Dep. Chem. Engineering, Beijing Inst. Technol.,

Beijing, 100081, Peop. Rep. China

SOURCE: Journal of Energetic Materials (1994), 12(4), 237-47

CODEN: JOEMDK; ISSN: 0737-0652

PUBLISHER: Dowden, Brodman & Devine, Inc.

DOCUMENT TYPE: Journal LANGUAGE: English

AB Three polyazido (nitro) stilbenes were prepared from polynitrostilbenes and sodium azide. Addition of 2 mol of this nucleophile to a solution of 3-chloro-2,2',4,4',6,6'-hexanitrostilbene in DMF resulted in the substitution of azido groups for one nitro group and the chlorine in the same benzene ring. The reactions of 2,2',4,4',6,6'-hexanitrostilbene with 2 and 4 mol of NaN3 exhibit a different reactivity and selectivity and produce sym. substituted azido polynitrostilbenes.

L21 ANSWER 13 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1994:110978 HCAPLUS

DOCUMENT NUMBER: 120:110978

TITLE: The compatibility of azido-plasticizers with binders AUTHOR(S): Yang, KeXi; Ding, FaXiang; Dai, XianYa; Tan, JingYu CORPORATE SOURCE: Xin Feng Chem. Eng. Inst., Shanghai, Peop. Rep. China Symposium on Chemical Problems Connected with the

OURCE: Symposium on Chemical Problems Connected with the Stability of Explosives, [Proceedings] (1993), 9th,

267-73

CODEN: SCPEDW; ISSN: 0348-7180

DOCUMENT TYPE: Journal LANGUAGE: English

AB Azido-type plasticizers can be used as energetic plasticizers in composite solid propellants because of their pos. heat of formation and high densities. Azido group-containing plasticizers like GAP can also form azido polymer-containing composite solid propellants when they become components of propellants. From weight loss tests at 80°, azido-oxypropylene dinitrate (AZP-2) and azido group-terminated polyazido
-oxypropylene (AZP-3), when mixed with binders, were chemical incompatible with unsatd. binders and cyano group-containing binders. Carboxylic acids can catalyze the decomposition of azides. The above plasticizers did not react with propylene oxide-butylene oxide copolymer, but they were also insol. in it.

L21 ANSWER 14 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1994:8208 HCAPLUS

DOCUMENT NUMBER: 120:8208

TITLE: Process for preparation of polyazido

11/17/2005

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alcohols from oxiranes, and preparation of derived

polyamino alcohols, polyazido thiols, and

cyclic ureas

INVENTOR(S):

Caubere, Paul; Forconi, Herve

PATENT ASSIGNEE(S): SOURCE:

Etat Francais, Fr. Can. Pat. Appl., 17 pp.

CODEN: CPXXEB

DOCUMENT TYPE:

Patent

LANGUAGE:

French

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CA 2083465	AA	19930522	CA 1992-2083465	19921120
FR 2684102	A1	19930528	FR 1991-14541	19911121
FR 2684102	B1	19940311		
US 5442080	Α	19950815	US 1992-980217	19921123
PRIORITY APPEN. INFO.:			FR 1991-14541 A	19911121
OTHER SÖÜRCE(S):	CASRE	ACT 120:8208;	MARPAT 120:8208	
GT		·		

$$R^{1}$$
 R^{2}
 R^{3}
 R^{4}

AB Various polyazido alcs. are prepared by reaction of oxiranes, e.g. I [X = nucleofugal substituent; R1 = H, (halo)alkyl, (un)substituted aryl; R2, R3 = H, (un) substituted alkyl or aryl; R4 = H, (un) substituted alkyl, (alkoxy)aryl], with a metal azide in an aqueous medium (56-93% yield). The azido alcs., e.g. diazido alcs. N3CR1R2CR4(OH)CHR3N3 or N3CR1R2CR4 (N3) CHR3OH, are hydrogenated to give the corresponding diamino alcs. (78-96%), which are cyclized with COCl2 to give cyclic ureas (93-98%). Alternatively, a diazido alc. may react with SOC12-pyridine (87%) and then NaSH-NaOH (40%) to give diazido thiols. Thus, reaction of 200 mmol NaN3 with 50 mmol epichlorohydrin in H2O at 80° in the presence of 10 mmol tricaprylmethylammonium chloride (preferred catalyst) gave 93% 1,3-diazido-2-propanol.

L21 ANSWER 15 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

1987:617094 HCAPLUS

DOCUMENT NUMBER:

107:217094

TITLE:

Polyazido esters

INVENTOR(S):

Frankel, Milton B.; Wilson, Edgar R.

PATENT ASSIGNEE(S):

Rockwell International Corp., USA

SOURCE:

U.S., 3 pp.

DOCUMENT TYPE:

CODEN: USXXAM

LANGUAGE:

Patent

FAMILY ACC. NUM. COUNT:

English

PATENT INFORMATION:

PATENT NO.

KIND APPLICATION NO.

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US 4683085 A 19870728 US 1985-766459 19850819 PRIORITY APPLN. INFO.: US 1985-766459 19850819

OTHER SOURCE(S): CASREACT 107:217094

GI

AB Azido esters XCH2C(CH2N3)2CH2O2CCH2CH2C(NO3)2 (I; X = N3, ONO2) and II, useful as energetic plasticizers for propellants (each N3 group adds apprx.85 kcal/mol energy to the system), were prepared from acid chlorides and pentaerythritol azides. A solution of (O2N)3CCH2CH2COCl, HOCH2C(CH2N3)3, and ClCH2CH2Cl was refluxed 70 h to give 91.9% I (X = N3).

L21 ANSWER 16 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1986:555611 HCAPLUS

DOCUMENT NUMBER: 105:155611

TITLE: Chemical case bond system with azido compound bonding

INVENTOR(S): Dehm, Henry C.

PATENT ASSIGNEE(S): Hercules Inc. , USA

SOURCE: U.S., 8 pp.

CODEN: USXXAM DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4604248	Α	19860805	US 1985-697094	19850131
PRIORITY APPLN. INFO.:			US 1985-697094	19850131

AB Solid propellants containing polyfunctional crosslinking components are bonded to rocket motor casings by the nitrene insertion reaction. Thin azido compound films, consisting of 1) a polyfunctional azido compound or polymer with crosslinker-reactive functionality for the propellant crosslinker and/or 2) a polyazido compound or polymer and a polyfunctional graftable compound or polymer having reactive functionality for the azido functionality and crosslinker-reactive functionality for the propellant crosslinker, are applied to the inner casing surface, energized to react the azide functionality with the insulator and graft the crosslinker-reactive functionality to the insulator surface, placing the propellant in contact with the grafted surface, and curing to react the propellant crosslinker with the functionality bonded to the insulator surface. Thus, EPDM insulator sheets are degreased and brush-coated with 1 part bis(β -azidoformyloxyethyl)isophthalate and 1 part 2-hydroxypropylcellulose in 15 parts acetone, the solvent is removed, the air temperature is raised to $140 \pm 3^{\circ}$ for 40 min, and the sheet is cooled, and placed into a matching polyethylene-coated cardboard carton. A standard isocyanate-cured slurry is cast 1 in. deep against the grafted surface and cured at 120°F. In tension, shear, and peel tests on the cured and machined product all failures were attributed to the propellant whereas controls made with ungrafted sheets failed at the

insulator-propellant interface. The effects of different curing conditions and of cellulose acetae butyrate, Hercules D-63 (a disulfonylazide), Et hydroxy cellulose, and bis(β -hydroxyethyl)isophthalate also are demonstrated.

L21 ANSWER 17 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1977:16869 HCAPLUS

DOCUMENT NUMBER: 86:16869

TITLE: Polynucleotides. XL. Synthesis and properties of

poly 2'-azido-2'-deoxyadenylic acid

AUTHOR(S): Ikehara, Morio; Fukui, Toshikazu; Kakiuchi, Nobuko

CORPORATE SOURCE: Fac. Pharm. Sci., Osaka Univ., Suita, Japan SOURCE: Nucleic Acids Research (1976), 3(8), 2089-99

CODEN: NARHAD; ISSN: 0305-1048

DOCUMENT TYPE: Journal LANGUAGE: English

AB Poly(2'-azido-2'-deoxyadenylic acid) (Poly Az) was synthesized from 2'-azido-2'-deoxyadenosine diphosphate by polynucleotide phosphorylase. Poly Az has uv absorption properties similar to poly A and hypochromicity of 40% at 0.1 M Na+ and neutrality. CD curve also resembled that of poly A with smaller ellipticity. Titration of poly Az with HCl gave a transition at pH 5.5, but the exact structure of the acid-form complex was not elucidated. Upon mixing with poly U, poly Az forms 1:1 and 1:2 complexes having melting temps. higher than that of poly A.poly U complex in the same condition.

L21 ANSWER 18 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1970:499592 HCAPLUS

DOCUMENT NUMBER: 73:99592

TITLE: Poly(azidoformamides), used as foaming agents in

polyolefins

INVENTOR(S): Suzuki, Shigeto
PATENT ASSIGNEE(S): Chevron Research Co.

SOURCE: U.S., 2 pp.
CODEN: USXXAM

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. _____ --------------US 1967-634138 19670427 US 1967-634138 A 19670427 US 3526644 Α 19700901 PRIORITY APPLN. INFO.: Poly(azidoformamides) (I), R(NHCON3)x, in which x = 2-4 and R is a polyvalent hydrocarbyl group, are prepared by treating a hydrocarbyl polyisocyanate with HN3, and are mixed with polyolefins and heated to form noncrosslinked foamed compns. Thus, a CHCl3 solution of NH3 was mixed with hexamethylene diisocyanate (II) to yield I (x = 2, R = hexamethylene), which was blended with polypropylene and poly(vinyl chloride) and heated to form noncrosslinked foamed polymers. m-Xylene, m-phenylene, and 4,4-diphenylmethane diisocyanate were also used instead of II, and produced similar foaming agents.

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